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(54) Title: CRYSTALLIZABLE COMPOSITIONS COMPRISING A HEPATITIS C VIRUS NS3 PROTEASE DOMAIN/NS4A COMPLEX AND CRYSTALS THEREBY OBTAINED
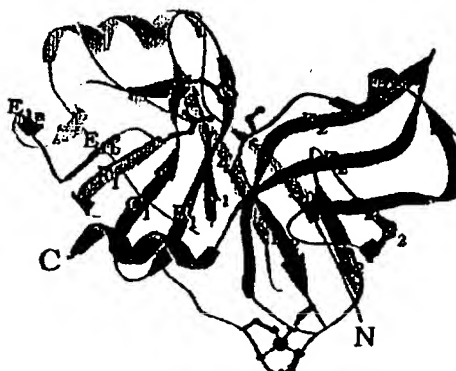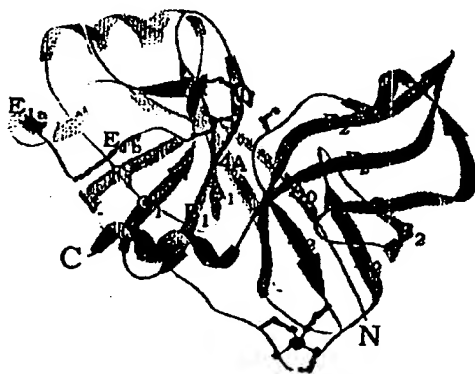
(57) Abstract

The present invention relates to compositions and crystals of a hepatitis C virus protease in complex with its viral cofactor. This invention also relates to methods of using the structure coordinates of hepatitis C virus protease in complex with a synthetic NS4A to solve the structure of similar or homologous proteins or protein complexes.

CRYSTALLIZABLE COMPOSITIONS COMPRISING A HEPATITIS C VIRUS NS3 PROTEASE DOMAIN/NS4A COMPLEX AND CRYSTALS THEREBY OBTAINED

5
TECHNICAL FIELD OF INVENTION

The present invention relates to compositions and crystals of a hepatitis C virus protease in complex with its viral cofactor. This invention also relates
10 to methods of using the structure coordinates of hepatitis C virus protease in complex with a synthetic NS4A to solve the structure of similar or homologous proteins or protein complexes.

15
BACKGROUND OF THE INVENTION

Infection by hepatitis C virus (HCV) is a compelling human medical problem. HCV is recognized as the causative agent for most cases of non-A, non-B
20 hepatitis, with an estimated human seroprevalence of 1% globally [Choo, Q.-L. et al., "Isolation of a cDNA Clone Derived From a Blood-Borne Non-A, Non-B Viral Hepatitis Genome", Science, 244, pp. 359-362 (1989); Kuo, G. et al., "An Assay for Circulating Antibodies to
25 a Major Etiologic Virus of Human Non-A, Non-B Hepatitis", Science, 244, pp. 362-364 (1989); Purcell, R.H., "Hepatitis C virus: Historical perspective and current concepts", FEMS Microbiology Reviews, 14, pp. 181-192 (1994); Van der Poel, C.L., "Hepatitis C Virus.
30 Epidemiology, Transmission and Prevention in Hepatitis C virus. Current Studies in Hematology and Blood Transfusion, H.W. Reesink, Ed., (Basel: Karger), pp. 137-163 (1994)]. Four million individuals may be

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infected in the United States alone [Alter, M.J. and
Mast, E.E., "The Epidemiology of Viral Hepatitis in
the United States, Gastroenterol. Clin. North Am., 23,
pp. 437-455 (1994)].

5   Upon first exposure to HCV only about 20% of
infected individuals develop acute clinical hepatitis
while others appear to resolve the infection
spontaneously. In most instances, however, the virus
establishes a chronic infection that persists for
10   decades [Iwarson, S. "The Natural Course of Chronic
Hepatitis", FEMS Microbiology Reviews, 14, pp. 201-204
(1994)]. This usually results in recurrent and
progressively worsening liver inflammation, which often
leads to more severe disease states such as cirrhosis
15   and hepatocellular carcinoma [Kew, M.C., "Hepatitis C
and Hepatocellular Carcinoma", FEMS Microbiology
Reviews, 14, pp. 211-220 (1994); Saito, I., et al.
"Hepatitis C Virus Infection is Associated with the
Development cf Hepatocellular Carcinoma", Proc. Natl.
20   Acad. Sci. USA 87, pp. 6547-6549 (1990)]. Currently,
there are no broadly effective treatments for the
debilitating progression of chronic HCV.

The HCV genome encodes a polyprotein of 3010-
3033 amino acids (Figure 1) [Choo, Q.-L., et al.
25   "Genetic Organization and Diversity of the Hepatitis C
Virus", Proc. Natl. Acad. Sci. USA, 88, pp. 2451-2455
(1991); Kato, N. et al., Molecular Cloning of the Human
Hepatitis C Virus Genome From Japanese Patients with
Non-A, Non-B Hepatitis", Proc. Natl. Acad. Sci. USA,
30   87, pp. 9524-9528 (1990); Takamizawa, A. et al.,
"Structure and Organization of the Hepatitis C Virus
Genome Isolated From Human Carriers", J. Virol., 65,
pp. 1105-1113 (1991)]. The HCV nonstructural (NS)

proteins provide catalytic machinery for viral
replication. The NS proteins are derived by
proteolytic cleavage of the polyprotein
[Bartenschlager, R. et al., "Nonstructural Protein 3 of
the Hepatitis C Virus Encodes a Serine-Type Proteinase
Required for Cleavage at the NS3/4 and NS4/5
Junctions", J. Virol., 67, pp. 3835-3844 (1993);
Grakoui, A. et al. "Characterization of the Hepatitis C
Virus-Encoded Serine Proteinase: Determination of
Proteinase-Dependent Polyprotein Cleavage Sites", J.
Virol., 67, pp. 2832-2843 (1993); Grakoui, A. et al.,
Expression and Identification of Hepatitis C Virus
Polyprotein Cleavage Products", J. Virol., 67, pp.
1385-1395 (1993); Tomei, L. et al., "NS3 is a serine
protease required for processing of hepatitis C virus
polyprotein", J. Virol., 67, pp. 4017-4026 (1993)].

      The HCV NS protein 3 (NS3) contains a serine
protease activity that helps process the majority of
the viral enzymes, and is thus considered essential for
viral replication and infectivity. It is known that
mutations in the yellow fever virus NS3 protease
decreases viral infectivity [Chambers, T.J. et. al.,
"Evidence that the N-terminal Domain of Nonstructural
Protein NS3 From Yellow Fever Virus is a Serine
Protease Responsible for Site-Specific Cleavages in the
Viral Polyprotein", Proc. Natl. Acad. Sci. USA, 87, pp.
8898-8902 (1990)]. The first 181 amino acids of NS3
(residues 1027-1207 of the viral polyprotein) have been
shown to contain the serine protease domain of NS3 that
processes all four downstream sites of the HCV
polyprotein (Figure 1) [C. Lin et al., "Hepatitis C
Virus NS3 Serine Proteinase: Trans-Cleavage

Requirements and Processing Kinetics", J. Virol., 68, pp. 8147-8157 (1994)].

NS3 is associated with a cofactor, NS4A. NS4A seems critical to the activity of NS3, enhancing the proteolytic efficiency of NS3 at all of the cleavage sites. NS4A is a 54 residue amphipathic peptide, with a hydrophobic N-terminus and a hydrophilic C-terminus [Failla, C. et al., "Both NS3 and NS4A are Required for Proteolytic Processing of Hepatitis C Virus Nonstructural Proteins", J. Virol., 68, pp. 3753-3760 (1994)]. Its function appears complex, possibly assisting in the membrane-localization of NS3 and other viral replicase components [Lin, C. et al. "A Central Region in the Hepatitis C Virus NS4A Protein Allows Formation of an Active NS3-NS4A Serine Proteinase Complex In Vivo and In Vitro", J. Virol., 69, pp. 4373-4380 (1995b); Shimizu, Y. et al., "Identification of the Sequence on NS4A Required for Enhanced Cleavage of the NS5A/5B Site by Hepatitis C Virus NS3 Protease", J. Virol., 70, pp. 127-132 (1996); Tanji, Y. et al., "Hepatitis C Virus-Encoded Nonstructural Protein NS4A has Versatile Functions in Viral Protein Processing", J. Virol., 69, pp. 1575-1581 (1995)] but its best characterized function is that of a cofactor for the NS3 protease.

The current understanding of HCV has not led to satisfactory treatments for HCV infection. The prospects for effective anti-HCV vaccines remain uncertain. The only established therapy for HCV disease is interferon treatment. However, interferons have significant side effects [Janssen, H. L. A., et al. "Suicide Associated with Alfa-Interferon Therapy for Chronic Viral Hepatitis", J. Hepatol., 21, pp. 241-

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243 (1994)]; Renault, P.F. and Hoofnagle, J.H., "Side
effects of alpha interferon. Seminars in Liver Disease
_9_, 273-277. (1989)] and induce long term remission in
only a fraction (~ 25%) of cases [Weiland, O.
5   "Interferon Therapy in Chronic Hepatitis C Virus
Infection", <u>FEMS Microbiol. Rev.</u>, 14, pp. 279-288
(1994)]. Thus, there is a need for more effective
anti-HCV therapies.

The NS3 protease is considered a potential
10   target for antiviral agents. However, drug discovery
efforts directed towards the NS3 protein have been
hampered by the lack of structural information about
NS3 and its complex with NS4A. Such structural
information would provide valuable information in
15   discovery of HCV NS3 protease inhibitors. However,
efforts to determine the structure of HCV NS3 protease
have been hampered by difficulties in obtaining
sufficient quantities of pure active enzyme
[Steinkuhler, C. et al., "In Vitro Activity of
20   Hepatitis C Virus Protease NS3 Purified from
Recombinant Baculovirus-Infected Sf9 Cells", <u>J. Biol
Chem.</u>, pp. 637-6273 (1996)]. There have been no
crystals reported of any NS3 or NS3 protease domain
protein. Thus, x-ray crystallographic analysis of such
25   proteins has not been possible.

SUMMARY OF THE INVENTION

Applicants have solved this problem by
30   providing, for the first time, compositions comprising
a hepatitis C virus (HCV) NS3 protease-like polypeptide
complexed with a NS4A-like peptide and methods for
making such compositions.

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The invention also provides crystals of a HCV NS3 protease-like polypeptide/NS4A-like peptide complex and methods for making such crystals.

The invention also provides the structure
5   coordinates of a HCV NS3 protease-like polypeptide/NS4A-like peptide complex.

The invention also provides a method for determining at least a portion of the three-dimensional structure of molecules or molecular complexes which
10   contain at least some structurally similar features to a HCV NS3 serine protease domain.

BRIEF DESCRIPTION OF THE FIGURES

15   Figure 1 depicts HCV polyprotein processing. The locations of the HCV structural and nonstructural proteins are marked on a diagram of the 3011 amino acid polypeptide. Cleavages between the structural proteins by cellular signal peptidases are marked by asterisks.
20   Cleavage between NS2 and NS3 is mediated by the NS2/NS3 metallo-protease. The NS3 serine protease is responsible for cleavages between NS3 and NS4A, NS4A and NS4B, NS4B and NS5A, and NS5A and NS5B.

Figure 2 depicts stereo ribbon diagrams of
25   the NS3/NS4A complex. The view is into the active site cleft of the enzyme. Side-chains of active site residues His-1083, Asp-1107, and Ser-1165, along with Zn^{++} ligands Cys-1123, Cys-1125, and Cys-1171 are displayed in ball-and-stick representation. Zn^{++}, its
30   H_2O ligand, and the β-strand formed by NS4A are also shown.

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Figure 3 lists the atomic structure coordinates for hepatitis C virus recombinant, truncated nonstructural protein 3 (hereafter referred to as tNS3) in complex with a synthetic peptide of the

5   central region of the nonstructural protein 4A (hereafter referred to as sNS4A) as derived by X-ray diffraction from crystals of that complex (hereafter referred to as tNS3/sNS4A). The preparation of the complex is described in Examples 1 and 2. The

10   following abbreviations are used in Figure 3:

"Atom type" refers to the element whose coordinates have been determined. Elements are defined by the first letter in the column except for zinc which is defined by the letters "Zn".

15   "X, Y, Z" crystallographically define the atomic position determined for each atom.

"B" is a thermal factor that measures movement of the atom around its atomic center.

"Occ" is an occupancy factor that refers to

20   the fraction of the molecules in which each atom occupies the position specified by the coordinates. A value of "1" indicates that each atom has the same conformation, i.e., the same position, in all molecules of the crystal.

25   Figure 4 shows a diagram of a system used to carry out the instructions encoded by the storage medium of Figures 5 and 6.

Figure 5 shows a cross section of a magnetic storage medium.

30   Figure 6 shows a cross section of a optically-readable data storage medium.

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DETAILED DESCRIPTION OF THE INVENTION

The following abbreviations are used throughout the application:

A	=	Ala	=	Alanine	T	=	Thr	=	Threonine

A = Ala = Alanine   T = Thr = Threonine

V = Val = Valine   C = Cys = Cysteine

L = Leu = Leucine   Y = Tyr = Tyrosine

I = Ile = Isoleucine   N = Asn = Asparagine

P = Pro = Proline   Q = Gln = Glutamine

F = Phe = Phenylalanine   D = Asp = Aspartic Acid

W = Trp = Tryptophan   E = Glu = Glutamic Acid

M = Met = Methionine   K = Lys = Lysine

G = Gly = Glycine   R = Arg = Arginine

S = Ser = Serine   H = His = Histidine

HCV = hepatitis C virus

Additional definitions are set forth in the
5   specification where necessary.

In order that the invention described herein
may be more fully understood, the following detailed
description is set forth.

Applicants have solved the above problems by
10   providing, for the first time, crystallizable
compositions comprising a HCV NS3 protease-like
polypeptide in complex with a NS4A-like peptide.

Thus, in one embodiment of this invention is
provided a composition comprising a hepatitis C virus
15   NS3-like polypeptide in complex with an NS4A-like
peptide.

The HCV NS3-like polypeptide portion of the
complex is any polypeptide which has the serine
protease activity of the naturally occurring HCV NS3A
20   protease, particularly the ability to cleave the HCV

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polyprotein. It includes HCV NS3, NS3 protease domain
polyprotein and NS3 protease domain-like polypeptides.

As used herein, the terms "HCV NS3" and "NS3"
refers to the hepatitis C virus nonstructural-3 protein
5   as defined in Lin, C. et al., "Hepatitis C Virus NS3
Serine Proteinase: *Trans*-Cleavage Requirements and
Processing Kinetics", J. Virol., 68, pp. 8147-8157
(1994).

The term "NS3 protease domain polypeptide"
10   refers to a truncated, serine protease portion of NS3
as defined in [Bartenschlager, R. et al.,
"Nonstructural Protein 3 of the Hepatitis C Virus
Encodes a Serine-Type Proteinase Required for Cleavage
at the NS3/4 and NS4/5 Junctions", J. Virol., 67, pp.
15   3835-3844 (1993); Grakoui, A. et al. "Characterization
of the Hepatitis C Virus-Encoded Serine Proteinase:
Determination of Proteinase-Dependent Polyprotein
Cleavage Sites", J. Virol., 67, pp. 2832-2843 (1993);
Grakoui, A. et al., Expression and Identification of
20   Hepatitis C Virus Polyprotein Cleavage Products", J.
Virol., 67, pp. 1385-1395 (1993); Tomei, L. et al.,
"NS3 is a serine protease required for processing of
hepatitis C virus polyprotein", J. Virol., 67, pp.
4017-4026 (1993)]. The disclosure of each of these
25   documents is herein incorporated by reference.

The term "NS3 protease domain-like
polypeptides" refers to polypeptides that differ from
NS3 protease domain polypeptides by having amino acid
deletions, substitutions, and additions, but which
30   retain the serine protease activity of NS3.

Preferably, the NS3-like polypeptide in the
compositions of this invention is tNS3, a recombinantly

produced hepatitis C virus protease domain protein that is prepared as described herein.

The NS4A-like peptide portion of the compositions of this invention is any peptide or peptide mimetic that is capable of acting as a NS4A cofactor for the NS3. These include NS4A, peptide fragments thereof and other peptides that differ from NS4A by having amino acid deletions, substitutions, and additions, while retaining the above-described activity.

As used herein the term "NS4A" refers to the hepatitis C virus nonstructural protein 4A which acts as a cofactor for NS3 protease [Failla, C. et al., "Both NS3 and NS4A are Required for Proteolytic Processing of Hepatitis C Virus Nonstructural Proteins" J. Virol. 68, pp. 3753-3760 (1994); Lin, C. et al., "Hepatitis C Virus NS3 Serine Proteinase: Trans-Cleavage Requirements and Processing Kinetics" J. Virol. 68, pp. 8147-8157 (1994b)]

Preferably, the NS4A-like peptide is sNS4A, the synthetic peptide H-KKGSVVIVGRIVLSGKPAIIPKK-OH. This peptide encompasses the essential NS3 protease domain residues of NS4A.

Both the NS3-like polypeptide and the NS4A-like peptide may be produced by any well-known method, including synthetic methods, such as solid phase, liquid phase and combination solid phase/liquid phase syntheses; recombinant DNA methods, including cDNA cloning, optionally combined with site directed mutagenesis; and/or purification of the natural products, optionally combined with enzymatic cleavage methods to produce fragments of naturally occurring NS3 and NS4A.

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According to a preferred embodiment, the
compositions of this invention are crystallizable. In
this preferred embodiment all of the preferred choices
for the NS3-like polypeptide and the NS4A-like peptide
5   are identical to those indicated above.

Advantageously, the crystallizable
composition provided by this invention are amenable to
x-ray crystallography. Thus, this invention also
provides the three-dimensional structure of an HCV NS3-
10   like polypeptide/NS4A-like peptide complex,
specifically an HCV tNS3/sNS4A complex, at 2.5 Å
resolution. Importantly, this has provided for the
first time, information about the shape and structure
of the NS3 protease domain.

15   The three-dimensional structure of the HCV
tNS3/sNS4A complex of this invention is defined by a
set of structure coordinates as set forth in Figure 3.
The term "structure coordinates" refers to Cartesian
coordinates derived from mathematical equations related
20   to the patterns obtained on diffraction of a
monochromatic beam of X-rays by the atoms (scattering
centers) of an tNS3/sNS4A complex in crystal form. The
diffraction data are used to calculate an electron
density map of the repeating unit of the crystal. The
25   electron density maps are then used to establish the
positions of the individual atoms of the tNS3/sNS4A
enzyme or enzyme complex.

Those of skill in the art will understand
that a set of structure coordinates for an enzyme or an
30   enzyme-complex or a portion thereof, is a relative set
of points that define a shape in three dimensions.
Thus, it is possible that an entirely different set of
coordinates could define a similar or identical shape.

Moreover, slight variations in the individual coordinates will have little effect on overall shape.

The variations in coordinates discussed above may be generated because of mathematical manipulations of the structure coordinates. For example, the structure coordinates set forth in Figure 3 could be manipulated by crystallographic permutations of the structure coordinates, fractionalization of the structure coordinates, integer additions or subtractions to sets of the structure coordinates, inversion of the structure coordinates or any combination of the above.

Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal could also account for variations in structure coordinates. If such variations are within an acceptable standard error as compared to the original coordinates, the resulting three-dimensional shape is considered to be the same.

Various computational analyses are therefore necessary to determine whether a molecule or molecular complex or a portion thereof is sufficiently similar to all or parts of the NS3-like polypeptide/NS4A-like peptide structure described above as to be considered the same. Such analyses may be carried out in current software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., San Diego, CA) version 4.1, and as described in the accompanying User's Guide.

The Molecular Similarity application permits comparisons between different structures, different

conformations of the same structure, and different
parts of the same structure. The procedure used in
Molecular Similarity to compare structures is divided
into four steps: 1) load the structures to be

5   compared; 2) define the atom equivalences in these
structures; 3) perform a fitting operation; and 4)
analyze the results.

Each structure is identified by a name. One
structure is identified as the target (i.e., the fixed

10   structure); all remaining structures are working
structures (i.e., moving structures). Since atom
equivalency within QUANTA is defined by user input, for
the purpose of this invention we will define equivalent
atoms as protein backbone atoms (N, Cα, C and O) for

15   all conserved residues between the two structures being
compared. We will also consider only rigid fitting
operations.

When a rigid fitting method is used, the
working structure is translated and rotated to obtain

20   an optimum fit with the target structure. The fitting
operation uses an algorithm that computes the optimum
translation and rotation to be applied to the moving
structure, such that the root mean square difference of
the fit over the specified pairs of equivalent atom is

25   an absolute minimum. This number, given in angstroms,
is reported by QUANTA.

For the purpose of this invention, any
molecule or molecular complex that has a root mean
square deviation of conserved residue backbone atoms

30   (N, Cα, C, O) of less than 1.5 Å when superimposed on
the relevant backbone atoms described by structure
coordinates listed in Figure 3 are considered

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identical. More preferably, the root mean square
deviation is less than 1.0 Å.

5   The term "root mean square deviation" means
the square root of the arithmetic mean of the squares
of the deviations from the mean. It is a way to
express the deviation or variation from a trend or
object. For purposes of this invention, the "root mean
square deviation" defines the variation in the backbone
of a protein or protein complex from the relevant
10   portion of the backbone of the NS3-like polypeptide
portion of the complex as defined by the structure
coordinates described herein.

Once the structure coordinates of a protein
crystal have been determined they are useful in solving
15   the structures of other crystals.

Thus, in accordance with the present
invention, the structure coordinates of a NS3-like
polypeptide/NS4A-like peptide complex, and in
particular a tNS3/sNS4A complex, and portions thereof
20   is stored in a machine-readable storage medium. Such
data may be used for a variety of purposes, such as
drug discovery and x-ray crystallographic analysis or
protein crystal.

Accordingly, in one embodiment of this
25   invention is provided a machine-readable data storage
medium comprising a data storage material encoded with
the structure coordinates set forth in Figure 3.

Figure 4 demonstrates one version of these
embodiments. System 10 includes a computer 11
30   comprising a central processing unit ("CPU") 20, a
working memory 22 which may be, e.g, RAM (random-access
memory) or "core" memory, mass storage memory 24 (such
as one or more disk drives or CD-ROM drives), one or

more cathode-ray tube ("CRT") display terminals 26, one
or more keyboards 28, one or more input lines 30, and
one or more output lines 40, all of which are
interconnected by a conventional bidirectional system

5   bus 50.

    Input hardware 36, coupled to computer 11 by
input lines 30, may be implemented in a variety of
ways. Machine-readable data of this invention may be
inputted via the use of a modem or modems 32 connected

10 by a telephone line or dedicated data line 34.
Alternatively or additionally, the input hardware 36
may comprise CD-ROM drives or disk drives 24. In
conjunction with display terminal 26, keyboard 28 may
also be used as an input device.

15   Output hardware 46, coupled to computer 11 by
output lines 40, may similarly be implemented by
conventional devices. By way of example, output
hardware 46 may include CRT display terminal 26 for
displaying a graphical representation of a binding

20 pocket of this invention using a program such as QUANTA
as described herein. Output hardware might also
include a printer 42, so that hard copy output may be
produced, or a disk drive 24, to store system output
for later use.

25   In operation, CPU 20 coordinates the use of
the various input and output devices 36, 46,
coordinates data accesses from mass storage 24 and
accesses to and from working memory 22, and determines
the sequence of data processing steps. A number of

30 programs may be used to process the machine-readable
data of this invention. Such programs are discussed in
reference to the computational methods of drug
discovery as described herein. Specific references to

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components of the hardware system 10 are included as
appropriate throughout the following description of the
data storage medium.

        Figure 5 shows a cross section of a magnetic
5   data storage medium 100 which can be encoded with a
machine-readable data that can be carried out by a
system such as system 10 of Figure 4. Medium 100 can
be a conventional floppy diskette or hard disk, having
a suitable substrate 101, which may be conventional,
10   and a suitable coating 102, which may be conventional,
on one or both sides, containing magnetic domains (not
visible) whose polarity or orientation can be altered
magnetically. Medium 100 may also have an opening (not
shown) for receiving the spindle of a disk drive or
15   other data storage device 24.

        The magnetic domains of coating 102 of medium
100 are polarized or oriented so as to encode in manner
which may be conventional, machine readable data such
as that described herein, for execution by a system
20   such as system 10 of Figure 4.

        Figure 6 shows a cross section of an
optically-readable data storage medium 110 which also
can be encoded with such a machine-readable data, or
set of instructions, which can be carried out by a
25   system such as system 10 of Figure 4. Medium 110 can
be a conventional compact disk read only memory
(CD-ROM) or a rewritable medium such as a
magneto-optical disk which is optically readable and
magneto-optically writable. Medium 100 preferably has
30   a suitable substrate 111, which may be conventional,
and a suitable coating 112, which may be conventional,
usually of one side of substrate 111.

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In the case of CD-ROM, as is well known, coating 112 is reflective and is impressed with a plurality of pits 113 to encode the machine-readable data. The arrangement of pits is read by reflecting laser light off the surface of coating 112. A protective coating 114, which preferably is substantially transparent, is provided on top of coating 112.

In the case of a magneto-optical disk, as is well known, coating 112 has no pits 113, but has a plurality of magnetic domains whose polarity or orientation can be changed magnetically when heated above a certain temperature, as by a laser (not shown). The orientation of the domains can be read by measuring the polarization of laser light reflected from coating 112. The arrangement of the domains encodes the data as described above.

For the first time, the present invention permits the use of structure-based or rational drug design techniques to design, select, and synthesize chemical entities, including inhibitory compounds that are capable of binding to HCV NS3, NS4A, NS3/NS4A complex, or any portion thereof.

One particularly useful drug design technique enabled by this invention is iterative drug design. Iterative drug design is a method for optimizing associations between a protein and a compound by determining and evaluating the three-dimensional structures of successive sets of protein/compound complexes.

Those of skill in the art will realize that association of natural ligands or substrates with the binding pockets of their corresponding receptors or

enzymes is the basis of many biological mechanisms of action. The term "binding pocket", as used herein, refers to a region of a molecule or molecular complex, that, as a result of its shape, favorably associates

5   with another chemical entity or compound. Similarly, many drugs exert their biological effects through association with the binding pockets of receptors and enzymes. Such associations may occur with all or any parts of the binding pockets. An understanding of such

10   associations will help lead to the design of drugs having more favorable associations with their target receptor or enzyme, and thus, improved biological effects. Therefore, this information is valuable in designing potential ligands or inhibitors of receptors

15   or enzymes, such as inhibitors of HCV NS3-like polypeptides, and more importantly HCV NS3.

The term "associating with" refers to a condition of proximity between chemical entities or compounds, or portions thereof. The association may be

20   non-covalent -- wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions -- or it may be covalent.

In iterative drug design, crystals of a

25   series of protein/compound complexes are obtained and then the three-dimensional structures of each complex is solved. Such an approach provides insight into the association between the proteins and compounds of each complex. This is accomplished by selecting compounds

30   with inhibitory activity, obtaining crystals of this new protein/compound complex, solving the three-dimensional structure of the complex, and comparing the associations between the new protein/compound complex

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and previously solved protein/compound complexes.   By
observing how changes in the compound affected the
protein/compound associations, these associations may
be optimized.

5   In some cases, iterative drug design is
carried out by forming successive protein-compound
complexes and then crystallizing each new complex.
Alternatively, a pre-formed protein crystal is soaked
in the presence of an inhibitor, thereby forming a

10   protein/compound complex and obviating the need to
crystallize each individual protein/compound complex.
Advantageously, the HCV NS3-like polypeptide/NS4A-like
peptide crystals, and in particular the tNS3/sNS4A
crystals, provided by this invention may be soaked in

15   the presence of a compound or compounds, such as NS3
protease inhibitors, to provide NS3-like
polypeptide/NS4A-like peptide /compound crystal
complexes.

           As used herein, the term "soaked" refers to a

20   process in which the crystal is transferred to a
solution containing the compound of interest.

           In another embodiment of this invention is
provided a method for preparing a composition
comprising a NS3-like polypeptide protein comprising

25   the steps described in Examples 1 and 2. Preferably,
the composition comprises a NS3-like polypeptide in
complex with a NS4A-like peptide.

           The structure coordinates set forth in Figure
3 can also be used to aid in obtaining structural

30   information about another crystallized molecule or
molecular complex. This may be achieved by any of a
number of well-known techniques, including molecular
replacement.

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The structure coordinates set forth in Figure 3 can also be used for determining at least a portion of the three-dimensional structure of molecules or molecular complexes which contain at least some

5   structurally similar features to HCV NS3. In particular, structural information about another crystallized molecule or molecular complex may be obtained. This may be achieved by any of a number of well-known techniques, including molecular replacement.

10   Therefore, in another embodiment this invention provides a method of utilizing molecular replacement to obtain structural information about a crystallized molecule or molecular complex whose structure is unknown comprising the steps of:

15   a) generating an X-ray diffraction pattern from said crystallized molecule or molecular complex; and

b) applying at least a portion of the structure coordinates set forth in Figure 3 to the

20   X-ray diffraction pattern to generate a three-dimensional electron density map of the molecule or molecular complex whose structure is unknown.

Preferably, the crystallized molecule or molecular complex comprises a NS3-like polypeptide and

25   a NS4A-like peptide. More preferably, the crystallized molecule or molecular complex is obtained by soaking a crystal of this invention in a solution.

By using molecular replacement, all or part of the structure coordinates of the tNS3/sNS4A complex

30   provided by this invention (and set forth in Figure 3) can be used to determine the structure of a crystallized molecule or molecular complex whose structure is unknown more quickly and efficiently than attempting to determine such information ab initio.

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Molecular replacement provides an accurate estimation of the phases for an unknown structure. Phases are a factor in equations used to solve crystal structures that can not be determined directly.

5   Obtaining accurate values for the phases, by methods other than molecular replacement, is a time-consuming process that involves iterative cycles of approximations and refinements and greatly hinders the solution of crystal structures. However, when the

10   crystal structure of a protein containing at least a homologous portion has been solved, the phases from the known structure provide a satisfactory estimate of the phases for the unknown structure.

Thus, this method involves generating a

15   preliminary model of a molecule or molecular complex whose structure coordinates are unknown, by orienting and positioning the relevant portion of the tNS3/sNS4A complex according to Figure 3 within the unit cell of the crystal of the unknown molecule or molecular

20   complex so as best to account for the observed X-ray diffraction pattern of the crystal of the molecule or molecular complex whose structure is unknown. Phases can then be calculated from this model and combined with the observed X-ray diffraction pattern amplitudes

25   to generate an electron density map of the structure whose coordinates are unknown. This, in turn, can be subjected to any well-known model building and structure refinement techniques to provide a final, accurate structure of the unknown crystallized molecule

30   or molecular complex [E. Lattman, "Use of the Rotation and Translation Functions", in Meth. Enzymol., 115, pp. 55-77 (1985); M. G. Rossmann, ed., "The Molecular Replacement Method", Int. Sci. Rev. Ser., No. 13, Gordon & Breach, New York (1972)].

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The structure of any portion of any
crystallized molecule or molecular complex that is
sufficiently homologous to any portion of the
tNS3/sNS4A complex can be solved by this method.

5   In a preferred embodiment, the method of
molecular replacement is utilized to obtain structural
information about a molecule or molecular complex,
wherein the complex comprises a NS3-like polypeptide.
Preferably the NS3-like polypeptide is tNS3 or

10   homologue thereof.

The structure coordinates of tNS3/sNS4A as
provided by this invention are particularly useful in
solving the structure of other crystal forms of NS3-
like polypeptide, preferably other crystal forms of

15   tNS3; NS3-like polypeptide/NS4A-like peptide,
preferably tNS3/sNS4A; or complexes comprising any of
the above.

The structure coordinates are also
particularly useful to solve the structure of crystals

20   of NS3-like polypeptide/NS4A-like peptide complexes,
particularly tNS3/sNS4A, co-complexed with a variety of
chemical entities. This approach enables the
determination of the optimal sites for interaction
between chemical entities, including interaction of

25   candidate NS3 inhibitors with NS3 or the NS3/NS4A
complex. For example, high resolution X-ray
diffraction data collected from crystals exposed to
different types of solvent allows the determination of
where each type of solvent molecule resides. Small

30   molecules that bind tightly to these sites can then be
designed and synthesized and tested for their NS3
inhibition activity.

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All of the complexes referred to above may be studied using well-known X-ray diffraction techniques and may be refined versus 1.5-3 Å resolution X-ray data to an R value of about 0.20 or less using computer
5   software, such as X-PLOR [Yale University, ©1992, distributed by Molecular Simulations, Inc.; see, e.g., Blundell & Johnson, supra; Meth. Enzymol., vol. 114 & 115, H. W. Wyckoff et al., eds., Academic Press (1985)]. This information may thus be used to optimize
10   known NS3 inhibitors, and more importantly, to design new NS3 inhibitors.

In order that this invention be more fully understood, the following examples are set forth. These examples are for the illustrative purposes only
15   and are not to be construed as limiting the scope of this invention in any way.

EXAMPLE 1
Expression and Purification of tNS3

20   The truncated NS3 serine protease domain (tNS3) was cloned from a cDNA of the hepatitis C virus H strain [Grakoui, A. et al., "Expression and Identification of Hepatitis C Virus Polyprotein Cleavage Products", J. Virol., 67, pp. 1385-1395
25   (1993)]. The first 181 amino acids of NS3 (residues 1027-1207 of the viral polyprotein) have been shown to contain the serine protease domain of NS3 that processes all four downstream sites of the HCV polyprotein [Lin, C., et al., Hepatitis C Virus NS3
30   Serine Proteinase: *Trans*-Cleavage Requirements and Processing Kinetics", J. Virol. 68, pp. 8147-8157 (1994b)], so we expressed a $(His)_6$-fusion protein based on this tNS3. The plasmid pET-BS(+)/HCV/T7-$NS3_{181}$-His

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was derived from pTM3/HCV/1027-1207 (NS3$_{181}$) (Id.), by
using polymerase chain reaction to introduce epitope
tags and new restriction sites. A T7-tag (ASMTGGQQMG),
from the N-terminus of the gene 10 protein of the T7

5   bacteriophage
[Tsai, D.E. et al., "*In Vitro* Selection of an RNA
Epitope Immunologically Cross-Reactive With a Peptide",
Proc. Natl. Acad. Sci. USA, 89, pp. 8864-8868 (1992)],
was placed at the N-terminus of the tNS3 domain.   Two

10   linker residues (GS) were placed at the tNS3 C-
terminus, followed by the (His)$_6$-tag.   *E.coli*
JM109(DE3) cells, freshly transformed with the pET-
BS(+)/HCV/T7-NS3$_{181}$-His plasmid, were grown at 37 °C in
complex media supplement with 100 μg/ml ampicillin, in

15   a 10 L fermentor (Braun).   When the cell density
reached an OD$_{600}$ of 3-4 the temperature of the culture
was rapidly reduced to 30 °C, and induction was
immediately initiated by the addition of 1 mM IPTG.
Cells were harvested at 2 h post-induction, and flash

20   frozen at -70 °C prior to purification.
The tNS3 was purified from the soluble
fraction of the recombinant *E.coli* lysates as follows,
with all procedures being performed at 4 °C unless
stated otherwise.   Cell paste (75-100g) was resuspended

25   in 15 volumes of 50 mM HEPES, 0.3 M NaCl, 10% glycerol,
0.1% ß-octyl glucoside, 2 mM ß-mercaptoethanol, pH 8.0.
Cells were ruptured using a microfluidizer and the
homogenate was clarified by centrifugation at 100,000 x
g for 30 min.   The supernatant was brought to 50 mM

30   HEPES, 20 mM imidazole, 0.3 M NaCl, 27.5% glycerol,
0.1% ß-octyl- glucoside, 2 mM ß-mercaptoethanol, pH
8.0, and applied at 1.0 ml/min to a 7.0 ml Ni-Agarose

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affinity column, equilibrated in the same buffer.
After loading, the column was washed with 10-15 volumes
of equilibration buffer and the bound proteins were
eluted with equilibration buffer containing 0.35 M
5   imidazole. The protein was then size-fractionated on
two columns in series (each 2.6 cm x 90 cm) packed with
Pharmacia high resolution S100 resin and equilibrated
with 25 mM HEPES, 0.3M NaCl, 10% glycerol, 0.1% ß-
octylglucoside, 2 mM ß-mercaptoethanol, pH 8.0. The
10   tNS3 fractions, identified by SDS-PAGE, were pooled and
concentrated to 1 mg/ml using a Amicon Centriprep-10,
and stored at -70°C. The tNS3 was thawed slowly on ice
and the NS4A peptide (dissolved in the size-exclusion
chromatography buffer) was added at a tNS3:NS4A-peptide
15   molar ratio of 1:2. The sample was then diluted 2.5-
fold with 15 mM MES, 0.5 M NaCl, 20 mM ß-
mercaptoethanol, pH6.5, and concentrated to ~2 ml (~ 2
mg/ml) by ultrafiltration. The sample was then diluted
2-fold with the pH 6.5 buffer and concentrated again to
20   ~2 ml. This dilution process was repeated until it
gave a >40-fold dilution of the original buffer
constituents. The protein sample was then concentrated
to 13.0 mg/ml and centrifuged at ~300,000 x g for 20
min at 4 °C. Concentrations of the pure tNS3 and
25   tNS3/4A complex were determined by UV absorption
spectroscopy, using a molar absorption coefficient
(A_{280}) of 17,700 $M^{-1} \cdot cm^{-1}$.

EXAMPLE 2

30   ### 4A Peptide Synthesis and Purification
The HCV NS4A peptide was synthesized to span
residues Gly21 to Pro39 of the viral cofactor (residues

1678 to 1696 of the HCV polyprotein), which incorporates the essential region reported to be essential for NS3 stimulation [Lin, C. et al. "A Central Region in the Hepatitis C Virus NS4A Protein

5   Allows Formation of an Active NS3-NS4A Serine Proteinase Complex _In Vivo_ and _In Vitro_", _J. Virol._ 69, pp. 4373-4380 (1995)]. Lysine residues were added to the termini to assist aqueous solubility, and a serine residue was substituted for Cys22 (residue 1679 of the

10 polyprotein of the HCV H strain). The peptide (H-KKGSVVIVGRIVLSGKPAIIPKK-OH · TFA salt) was prepared by the solid-phase peptide synthesis (Applied Biosystems 433A) beginning with N^a-Fmoc, N^e-Boc-Lys Wang resin. N^a-Fmoc-protected amino acids were added sequentially

15 using HBTU (2-(1H-benzotriazol-1-yl)1,1,3,3-tetramethyluronium hexafluorophosphate) with HOBt (1-hydroxybenzotriazole hydrate) as coupling agents in N-methylpyrrolidinone. Cleavage from the resin and global deprotection were accomplished with 95%

20 trifluoroacetic acid and 5% water at room temperature for 1.5 hr (15 ml/ g resin). The peptide was purified by preparative HPLC on a Waters Delta Pak C18, 15 μm, 300Å column (30 mm x 300 mm) eluting with a linear gradient of acetonitrile (15-40%) in 0.1% aqueous

25 trifluoroacetic acid over 35 min (flow rate of 22 ml/min). Peptide purity was confirmed by analytical HPLC. The sequence was confirmed by direct N-terminal sequence analysis and matrix-assisted laser desorption mass spectrometry (Kratos MALDI I), which showed the

30 correct $(M + H)^+$ and $(M + Na)^+$ molecular ions.

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EXAMPLE 3
Crystallization and Data Collection

Crystals of the tNS3/NS4A complex were grown by hanging-drop vapor diffusion over a reservoir of 0.1 M MES, 1.8 M NaCl, 0.1 M sodium/potassium phosphate, 10 mM ß-mercaptoethanol, pH 6.5. The crystals grew over the course of 2-3 weeks, to final dimensions of about 0.1 x 0.1 x 0.25 mm. The rhombohedral crystals used in this study belonged to space group R32, with unit cell dimensions a=b=225.0Å, and c=75.5Å, and contained two tNS3/NS4A complexes per asymmetric unit.

Statistics for data collection, heavy atom refinement, and crystallographic refinement are given in Table 1. All heavy atom soaks were done in hanging-drops over the same reservoir as used for crystallization. Crystals were transferred to a stabilizing solution (50 mM MES, 2.0 M NaCl, 0.1 M sodium/potassium phosphate, 10 mM ß-mercaptoethanol, and 20% glycerol, pH 6.2) and then frozen in a dry nitrogen gas stream at 100 K (Molecular Structure Corp., Houston, TX) for data collection. Data was acquired by oscillation photography on a Rigaku R-AXIS IIC phosphor imaging area detector mounted on a Rigaku RU200 rotating anode generator (MSC), operating at 50kV and 100mA. Measured intensities were integrated, scaled, and merged using the HKL software package (Z. Otwinowski and W. Minor).

EXAMPLE 4
Phasing, Model Building and Refinement

Heavy atom positions were located by inspection and confirmed with difference Fourier syntheses. Heavy atom parameters were refined and

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phases computed to 3.1Å using the program PHASES
[Furey, W. and Swaminathan, S. "PHASES-95: a program
package for the processing and analysis of diffraction
data from macromolecules", Meth. Enzymol., (1996). MIR

5   phases were improved and extended to 2.7Å by cycles of
solvent flattening [Wang, B.C., "Resolution of Phase
Ambiguity in Macromolecular Crystallography", Methods
in Enzymol. 115, pp. 90-112 (1985)] combined with
histogram matching [Zhang, K.Y.J. and Main, P., "The

10   Use of Sayre's Equation With Solvent Flattening and
Histogram Matching for Phase Extension and Refinement
of Protein Structures", Acta Crystallogr., A46, pp.
377-381 (1990)] using the CCP4 crystallographic package
(Collaborative Computation Project, 1994). The

15   resulting electron density map displayed nearly
continuous density for the protein backbone as well as
strong side chain density. Approximately 80% of the
model could be unambiguously built into this map
(QUANTA 4.1, Molecular Simulations), and a single round

20   of simulated annealing refinement in X-PLOR [Brunger,
A. T., "X-PLOR: A System for X-Ray Crystallography and
NMR", New Haven, Connecticut: Department of Molecular
Biophysics and Biochemistry, Yale University (1993)]
brought the R-factor to 29% and free R value to 33%

25   [Brunger, A. T., "Free R Value: A Novel Statistical
Quantity for Assessing the Accuracy of Crystal
Structures", Nature, 355, pp. 472-475 (1992)]. The
remainder of the model was built and refined in several
steps, by first extending the resolution to 2.5Å and

30   then adding well-ordered water molecules. A final
round of positional and individual temperature factor
refinement brought the R-factor to 21.6% (free R value
26.1%) for 26,652 reflections between 6.0 and 2.5Å

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(F>1sF). The current model consisted of tNS3 residues 1055-1206 and NS4A residues 1678-1693 in complex A, and tNS3 residues 1028-1206 and NS4A residues 1678-1696 for complex B (polyprotein numbering, with 2 zinc atoms and 130 water molecules. A Ramachandran plot for the final model contained 91% of the residues in the most favored regions and 0% in disallowed or generously-allowed regions. The rms deviations from ideality were 0.007Å for bond lengths and 1.47° for bond angles.

While we have described a number of embodiments of this invention, it is apparent that our basic examples may be altered to provide other embodiments which utilize the products and processes of this invention. Therefore, it will be appreciated that the scope of this invention is to be defined by the appended claims rather than by the specific embodiments which have been represented by way of example.

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CLAIMS

We claim:

1.   A composition comprising a HCV NS3-like
polypeptide complexed with a NS4A-like peptide.

2.   The composition according to claim 1,
wherein the HCV NS3-like polypeptide is a NS3 protease
domain polypeptide or a NS3 protease domain-like
polypeptide.

3.   The composition according to claim 1,
wherein the HCV NS3-like polypeptide is tNS3.

4.   The composition according to any one of
claims 1 to 3, wherein the NS4A-like peptide is H-
KKGSVVIVGRIVLSGKPAIIPKK-OH.

5.   A crystal comprising a HCV NS3-like
polypeptide complexed with a NS4A-like peptide.

6.   The crystal according to claim 5, wherein
the HCV NS3-like polypeptide is a NS3 protease domain
polypeptide or a NS3 protease domain-like polypeptide.

7.   The crystal according to claim 5, wherein
the HCV NS3-like polypeptide is tNS3.

8.   The crystal according to any one of
claims 1 to 3, wherein the NS4A-like peptide is H-
KKGSVVIVGRIVLSGKPAIIPKK-OH.

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9.   The crystal according to claim 5,
additionally comprising an inhibitor of HVC NS3.

5   10.   A machine-readable data storage medium,
comprising a data storage material encoded with machine
readable data, wherein the data is defined by the
structure coordinates of a tNS3/sNS4A complex according
to Figure 3, or a homologue of said complex, wherein
said homologue comprises backbone atoms that have a
10   root mean square deviation from the backbone atoms of
the complex of not more than 1.5A

11.   The machine-readable data storage
medium, according to claim 10, wherein said molecule or
15   molecular complex is defined by the set of structure
coordinates for tNS3/sNS4A according to Figure 3, or a
homologue of said molecule or molecular complex, said
homologue having a root mean square deviation from the
backbone atoms of said amino acids of not more than 1.5
20   Ä.

12.   A machine-readable data storage medium
comprising a data storage material encoded with a first
set of machine readable data comprising a Fourier
25   transform of at least a portion of the structural
coordinates for tNS3/sNS4A according to Figure 3;
which, when combined with a second set of machine
readable data comprising an X-ray diffraction pattern
of a molecule or molecular complex of unknown
30   structure, using a machine programmed with instructions
for using said first set of data and said second set of
data, can determine at least a portion of the structure
coordinates corresponding to the second set of machine

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readable data, said first set of data and said second
set of data.

13.   A method of obtaining structural
information about a molecule or a molecular complex of
unknown structure by using the structure coordinates
set forth in Figure 3, comprising the steps of:
          a.   generating X-ray diffraction data from
said crystallized molecule or molecular complex;
          b.   applying at least a portion of the
structure coordinates set forth in Figure 3 to said
X-ray diffraction pattern to generate a
three-dimensional electron density map of at least a
portion of the molecule or molecular complex.

14.   The method according to claim 13,
wherein the molecule or molecular complex of unknown
structure comprises a polypeptide selected from a NS3-
like polypeptide in complex with a NS4A-like peptide.

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Fig. 1

Figure 2

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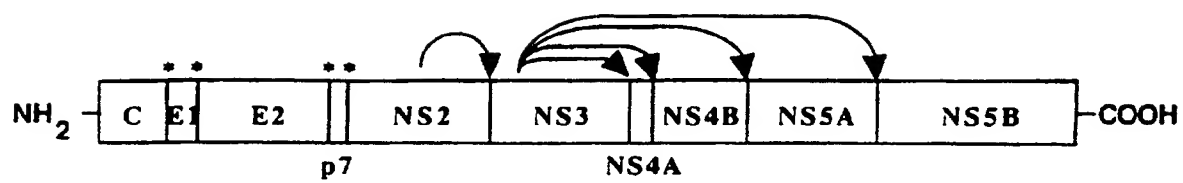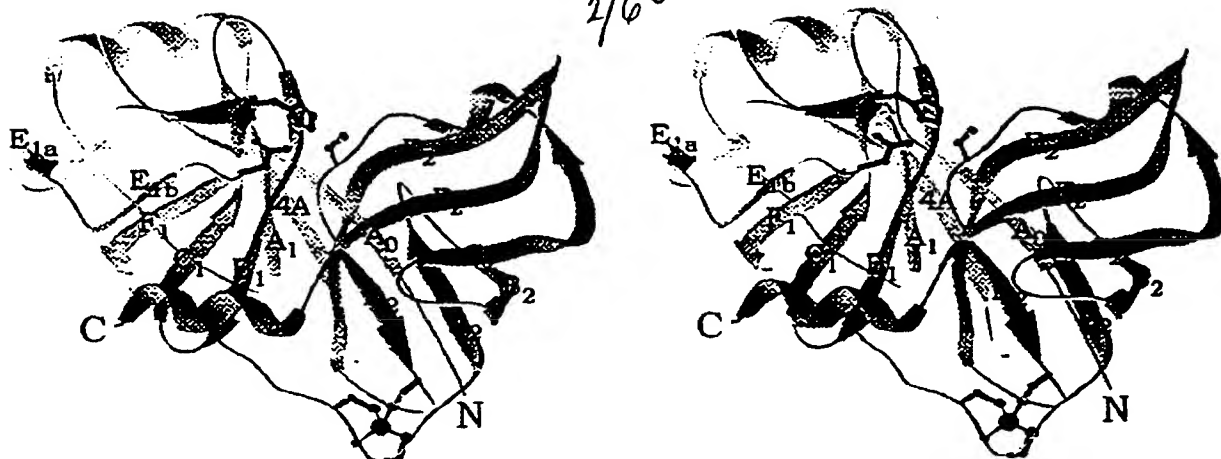
FIGURE 3

tNS3 COORDINATES   (Complex A)

|		Atom Type	Resid	#	X	Y	Z	OCC	B
ATOM	1	N	VAL	1055	94.186	42.391	51.819	1.00	32.85
ATOM	2	CA	VAL	1055	92.743	42.519	51.462	1.00	30.82
ATOM	3	CB	VAL	1055	92.435	41.883	50.083	1.00	30.41
ATOM	4	CG1	VAL	1055	90.953	41.986	49.767	1.00	31.38
ATOM	5	CG2	VAL	1055	93.232	42.576	48.999	1.00	30.52
ATOM	6	C	VAL	1055	91.928	41.817	52.527	1.00	30.32
ATOM	7	O	VAL	1055	92.271	40.715	52.954	1.00	31.39
ATOM	8	N	GLU	1056	90.869	42.481	52.975	1.00	30.38
ATOM	9	CA	GLU	1056	89.985	41.933	53.994	1.00	28.82
ATOM	10	CB	GLU	1056	89.909	42.877	55.191	1.00	28.56
ATOM	11	CG	GLU	1056	91.249	43.090	55.856	1.00	33.65
ATOM	12	CD	GLU	1056	91.183	44.066	57.007	1.00	37.88
ATOM	13	OE1	GLU	1056	91.610	43.695	58.120	1.00	40.68
ATOM	14	OE2	GLU	1056	90.713	45.204	56.796	1.00	40.04
ATOM	15	C	GLU	1056	88.590	41.675	53.442	1.00	26.54
ATOM	16	O	GLU	1056	88.102	42.417	52.591	1.00	26.63
ATOM	17	N	GLY	1057	87.970	40.602	53.914	1.00	24.45
ATOM	18	CA	GLY	1057	86.633	40.261	53.478	1.00	22.13
ATOM	19	C	GLY	1057	85.614	40.570	54.553	1.00	21.95
ATOM	20	O	GLY	1057	85.918	40.510	55.742	1.00	23.57
ATOM	21	N	GLU	1058	84.406	40.924	54.140	1.00	20.53
ATOM	22	CA	GLU	1058	83.352	41.236	55.084	1.00	18.51
ATOM	23	CB	GLU	1058	82.408	42.295	54.514	1.00	18.38
ATOM	24	CG	GLU	1058	83.060	43.597	54.096	1.00	18.99
ATOM	25	CD	GLU	1058	83.531	43.593	52.650	1.00	23.27
ATOM	26	OE1	GLU	1058	83.746	42.504	52.083	1.00	24.96
ATOM	27	OE2	GLU	1058	83.701	44.686	52.067	1.00	26.97
ATOM	28	C	GLU	1058	82.580	39.954	55.338	1.00	19.61
ATOM	29	O	GLU	1058	81.988	39.770	56.399	1.00	21.48
ATOM	30	N	VAL	1059	82.604	39.062	54.354	1.00	18.78
ATOM	31	CA	VAL	1059	81.899	37.789	54.428	1.00	18.22
ATOM	32	CB	VAL	1059	80.990	37.583	53.170	1.00	16.33
ATOM	33	CG1	VAL	1059	80.286	36.249	53.225	1.00	13.76
ATOM	34	CG2	VAL	1059	79.977	38.702	53.048	1.00	12.68
ATOM	35	C	VAL	1059	82.903	36.644	54.491	1.00	20.89
ATOM	36	O	VAL	1059	83.826	36.571	53.676	1.00	20.81
ATOM	37	N	GLN	1060	82.737	35.758	55.465	1.00	21.48
ATOM	38	CA	GLN	1060	83.629	34.620	55.582	1.00	22.32
ATOM	39	CB	GLN	1060	84.405	34.633	56.908	1.00	23.40
ATOM	40	CG	GLN	1060	83.662	35.176	58.104	1.00	24.97
ATOM	41	CD	GLN	1060	83.707	36.692	58.201	1.00	25.79
ATOM	42	OE1	GLN	1060	84.519	37.351	57.553	1.00	27.09
ATOM	43	NE2	GLN	1060	82.842	37.252	59.031	1.00	25.24
ATOM	44	C	GLN	1060	82.863	33.325	55.410	1.00	23.40
ATOM	45	O	GLN	1060	81.735	33.202	55.880	1.00	25.77

FIGURE 3 (CONT.)

ATOM	46	N	ILE	1061	83.457	32.399	54.663	1.00	23.80
ATOM	47	CA	ILE	1061	82.882	31.086	54.390	1.00	23.08
ATOM	48	CB	ILE	1061	83.399	30.530	53.052	1.00	23.13
ATOM	49	CG2	ILE	1061	82.659	29.258	52.698	1.00	20.59
ATOM	50	CG1	ILE	1061	83.219	31.584	51.951	1.00	23.17
ATOM	51	CD1	ILE	1061	83.949	31.275	50.692	1.00	21.52
ATOM	52	C	ILE	1061	83.335	30.173	55.517	1.00	24.42
ATOM	53	O	ILE	1061	84.498	29.766	55.574	1.00	26.06
ATOM	54	N	VAL	1062	82.404	29.850	56.404	1.00	25.24
ATOM	55	CA	VAL	1062	82.688	29.028	57.569	1.00	24.13
ATOM	56	CB	VAL	1062	82.085	29.682	58.832	1.00	21.93
ATOM	57	CG1	VAL	1062	82.568	31.124	58.951	1.00	20.61
ATOM	58	CG2	VAL	1062	80.578	29.645	58.778	1.00	18.03
ATOM	59	C	VAL	1062	82.201	27.587	57.443	1.00	26.46
ATOM	60	O	VAL	1062	81.391	27.261	56.573	1.00	26.50
ATOM	61	N	SER	1063	82.685	26.730	58.332	1.00	28.27
ATOM	62	CA	SER	1063	82.312	25.326	58.316	1.00	29.40
ATOM	63	CB	SER	1063	83.246	24.539	57.389	1.00	29.43
ATOM	64	OG	SER	1063	83.164	25.013	56.054	1.00	33.51
ATOM	65	C	SER	1063	82.339	24.684	59.696	1.00	31.16
ATOM	66	O	SER	1063	83.000	25.167	60.623	1.00	30.35
ATOM	67	N	THR	1064	81.593	23.593	59.811	1.00	33.89
ATOM	68	CA	THR	1064	81.497	22.790	61.023	1.00	33.81
ATOM	69	CB	THR	1064	80.091	22.855	61.651	1.00	31.40
ATOM	70	OG1	THR	1064	79.099	22.536	60.664	1.00	33.92
ATOM	71	CG2	THR	1064	79.825	24.230	62.216	1.00	29.94
ATOM	72	C	THR	1064	81.769	21.383	60.511	1.00	35.92
ATOM	73	O	THR	1064	81.951	21.200	59.305	1.00	36.71
ATOM	74	N	ALA	1065	81.800	20.395	61.396	1.00	38.38
ATOM	75	CA	ALA	1065	82.060	19.022	60.975	1.00	40.41
ATOM	76	CB	ALA	1065	82.104	18.114	62.181	1.00	41.57
ATOM	77	C	ALA	1065	81.044	18.490	59.966	1.00	41.85
ATOM	78	O	ALA	1065	81.357	17.623	59.151	1.00	41.76
ATOM	79	N	THR	1066	79.827	19.016	60.025	1.00	43.16
ATOM	80	CA	THR	1066	78.758	18.559	59.148	1.00	45.82
ATOM	81	CB	THR	1066	77.582	18.022	60.003	1.00	48.55
ATOM	82	OG1	THR	1066	77.141	19.047	60.914	1.00	51.57
ATOM	83	CG2	THR	1066	78.009	16.795	60.791	1.00	51.00
ATOM	84	C	THR	1066	78.147	19.613	58.224	1.00	46.64
ATOM	85	O	THR	1066	77.374	19.265	57.323	1.00	48.12
ATOM	86	N	GLN	1067	78.466	20.887	58.431	1.00	45.58
ATOM	87	CA	GLN	1067	77.829	21.923	57.636	1.00	43.33
ATOM	88	CB	GLN	1067	76.635	22.429	58.438	1.00	44.54
ATOM	89	CG	GLN	1067	75.606	23.244	57.682	1.00	48.92
ATOM	90	CD	GLN	1067	74.377	23.595	58.535	1.00	51.71
ATOM	91	OE1	GLN	1067	73.519	24.380	58.113	1.00	53.17
ATOM	92	NE2	GLN	1067	74.297	23.023	59.738	1.00	49.37
ATOM	93	C	GLN	1067	78.720	23.091	57.269	1.00	40.47
ATOM	94	O	GLN	1067	79.567	23.498	58.053	1.00	41.29
ATOM	95	N	THR	1068	78.523	23.612	56.063	1.00	37.11
ATOM	96	CA	THR	1068	79.261	24.767	55.574	1.00	30.70

FIGURE 3 (CONT.)

ATOM	97	CB	THR	1068	80.113	24.436	54.331	1.00	29.76
ATOM	98	OG1	THR	1068	81.008	25.521	54.062	1.00	30.04
ATOM	99	CG2	THR	1068	79.241	24.184	53.113	1.00	30.99
ATOM	100	C	THR	1068	78.236	25.843	55.234	1.00	28.68
ATOM	101	O	THR	1068	77.192	25.565	54.644	1.00	27.99
ATOM	102	N	PHE	1069	78.517	27.063	55.659	1.00	26.46
ATOM	103	CA	PHE	1069	77.631	28.186	55.420	1.00	23.03
ATOM	104	CB	PHE	1069	76.499	28.199	56.450	1.00	22.57
ATOM	105	CG	PHE	1069	76.955	27.964	57.854	1.00	22.39
ATOM	106	CD1	PHE	1069	77.011	29.014	58.759	1.00	22.57
ATOM	107	CD2	PHE	1069	77.351	26.699	58.271	1.00	22.33
ATOM	108	CE1	PHE	1069	77.458	28.808	60.057	1.00	23.82
ATOM	109	CE2	PHE	1069	77.800	26.485	59.566	1.00	22.79
ATOM	110	CZ	PHE	1069	77.855	27.543	60.461	1.00	23.30
ATOM	111	C	PHE	1069	78.456	29.472	55.447	1.00	22.55
ATOM	112	O	PHE	1069	79.670	29.421	55.249	1.00	21.97
ATOM	113	N	LEU	1070	77.832	30.607	55.734	1.00	19.95
ATOM	114	CA	LEU	1070	78.562	31.866	55.734	1.00	19.27
ATOM	115	CB	LEU	1070	78.091	32.748	54.571	1.00	19.20
ATOM	116	CG	LEU	1070	78.060	32.230	53.135	1.00	16.10
ATOM	117	CD1	LEU	1070	77.451	33.307	52.257	1.00	13.03
ATOM	118	CD2	LEU	1070	79.445	31.859	52.670	1.00	15.83
ATOM	119	C	LEU	1070	78.347	32.649	57.009	1.00	18.16
ATOM	120	O	LEU	1070	77.443	32.345	57.781	1.00	20.67
ATOM	121	N	ALA	1071	79.186	33.661	57.210	1.00	16.24
ATOM	122	CA	ALA	1071	79.091	34.565	58.349	1.00	17.10
ATOM	123	CB	ALA	1071	80.142	34.249	59.377	1.00	19.06
ATOM	124	C	ALA	1071	79.340	35.935	57.750	1.00	18.14
ATOM	125	O	ALA	1071	79.958	36.030	56.693	1.00	19.55
ATOM	126	N	THR	1072	78.839	36.981	58.396	1.00	17.51
ATOM	127	CA	THR	1072	78.999	38.345	57.909	1.00	16.67
ATOM	128	CB	THR	1072	77.679	38.890	57.335	1.00	14.90
ATOM	129	OG1	THR	1072	77.249	38.048	56.269	1.00	19.26
ATOM	130	CG2	THR	1072	77.852	40.303	56.799	1.00	13.79
ATOM	131	C	THR	1072	79.410	39.262	59.049	1.00	19.92
ATOM	132	O	THR	1072	78.785	39.264	60.112	1.00	22.53
ATOM	133	N	CYS	1073	80.470	40.032	58.840	1.00	20.00
ATOM	134	CA	CYS	1073	80.916	40.960	59.856	1.00	19.38
ATOM	135	CB	CYS	1073	82.388	41.267	59.691	1.00	17.15
ATOM	136	SG	CYS	1073	83.433	39.961	60.265	1.00	21.59
ATOM	137	C	CYS	1073	80.144	42.240	59.705	1.00	20.61
ATOM	138	O	CYS	1073	80.125	42.821	58.623	1.00	21.53
ATOM	139	N	ILE	1074	79.470	42.654	60.770	1.00	23.02
ATOM	140	CA	ILE	1074	78.706	43.903	60.793	1.00	24.61
ATOM	141	CB	ILE	1074	77.189	43.676	60.592	1.00	24.97
ATOM	142	CG2	ILE	1074	76.426	44.967	60.844	1.00	27.22
ATOM	143	CG1	ILE	1074	76.904	43.174	59.178	1.00	23.86
ATOM	144	CD1	ILE	1074	75.491	42.685	58.985	1.00	25.93
ATOM	145	C	ILE	1074	78.943	44.491	62.176	1.00	26.19
ATOM	146	O	ILE	1074	78.833	43.790	63.185	1.00	28.47
ATOM	147	N	ASN	1075	79.320	45.760	62.222	1.00	26.56

FIGURE 3 (CONT.)

ATOM	148	CA	ASN	1075	79.593	46.430	63.488	1.00	27.15
ATOM	149	CB	ASN	1075	78.297	46.703	64.261	1.00	28.70
ATOM	150	CG	ASN	1075	77.415	47.756	63.592	1.00	30.77
ATOM	151	OD1	ASN	1075	77.829	48.418	62.639	1.00	33.91
ATOM	152	ND2	ASN	1075	76.192	47.915	64.094	1.00	30.24
ATOM	153	C	ASN	1075	80.599	45.671	64.368	1.00	28.13
ATOM	154	O	ASN	1075	80.388	45.504	65.569	1.00	27.91
ATOM	155	N	GLY	1076	81.687	45.206	63.760	1.00	28.00
ATOM	156	CA	GLY	1076	82.723	44.506	64.502	1.00	27.37
ATOM	157	C	GLY	1076	82.411	43.101	64.970	1.00	29.01
ATOM	158	O	GLY	1076	83.264	42.433	65.567	1.00	28.27
ATOM	159	N	VAL	1077	81.205	42.631	64.678	1.00	29.05
ATOM	160	CA	VAL	1077	80.801	41.298	65.084	1.00	27.37
ATOM	161	CB	VAL	1077	79.453	41.339	65.821	1.00	26.61
ATOM	162	CG1	VAL	1077	79.062	39.956	66.292	1.00	27.45
ATOM	163	CG2	VAL	1077	79.536	42.281	66.995	1.00	27.61
ATOM	164	C	VAL	1077	80.688	40.392	63.864	1.00	27.94
ATOM	165	O	VAL	1077	80.387	40.852	62.759	1.00	29.66
ATOM	166	N	CYS	1078	80.989	39.114	64.062	1.00	26.17
ATOM	167	CA	CYS	1078	80.910	38.114	63.011	1.00	23.77
ATOM	168	CB	CYS	1078	82.097	37.158	63.101	1.00	23.73
ATOM	169	SG	CYS	1078	82.221	35.981	61.746	1.00	23.84
ATOM	170	C	CYS	1078	79.610	37.378	63.286	1.00	23.02
ATOM	171	O	CYS	1078	79.533	36.557	64.200	1.00	24.11
ATOM	172	N	TRP	1079	78.576	37.726	62.534	1.00	21.24
ATOM	173	CA	TRP	1079	77.260	37.133	62.698	1.00	19.55
ATOM	174	CB	TRP	1079	76.187	38.178	62.406	1.00	19.32
ATOM	175	CG	TRP	1079	76.340	39.431	63.178	1.00	21.82
ATOM	176	CD2	TRP	1079	75.766	39.721	64.460	1.00	23.32
ATOM	177	CE2	TRP	1079	76.112	41.055	64.781	1.00	24.08
ATOM	178	CE3	TRP	1079	74.989	38.986	65.364	1.00	21.58
ATOM	179	CD1	TRP	1079	77.003	40.560	62.788	1.00	22.05
ATOM	180	NE1	TRP	1079	76.868	41.542	63.745	1.00	23.78
ATOM	181	CZ2	TRP	1079	75.703	41.670	65.967	1.00	22.89
ATOM	182	CZ3	TRP	1079	74.582	39.596	66.540	1.00	22.78
ATOM	183	CH2	TRP	1079	74.940	40.929	66.831	1.00	23.44
ATOM	184	C	TRP	1079	77.028	35.976	61.763	1.00	18.27
ATOM	185	O	TRP	1079	77.576	35.939	60.661	1.00	20.23
ATOM	186	N	THR	1080	76.196	35.041	62.200	1.00	17.65
ATOM	187	CA	THR	1080	75.813	33.895	61.391	1.00	18.57
ATOM	188	CB	THR	1080	76.917	32.826	61.319	1.00	18.31
ATOM	189	OG1	THR	1080	76.535	31.806	60.384	1.00	15.58
ATOM	190	CG2	THR	1080	77.164	32.212	62.666	1.00	16.32
ATOM	191	C	THR	1080	74.506	33.321	61.930	1.00	19.72
ATOM	192	O	THR	1080	73.939	33.844	62.894	1.00	20.69
ATOM	193	N	VAL	1081	74.023	32.258	61.304	1.00	22.55
ATOM	194	CA	VAL	1081	72.767	31.633	61.700	1.00	23.39
ATOM	195	CB	VAL	1081	72.019	31.058	60.473	1.00	21.81
ATOM	196	CG1	VAL	1081	71.432	32.176	59.648	1.00	19.45
ATOM	197	CG2	VAL	1081	72.972	30.227	59.617	1.00	22.36
ATOM	198	C	VAL	1081	72.942	30.524	62.729	1.00	25.42

ATOM	199	O	VAL	1081	73.693	29.565	62.510	1.00	27.35
ATOM	200	N	TYR	1082	72.191	30.632	63.823	1.00	27.30
ATOM	201	CA	TYR	1082	72.211	29.644	64.902	1.00	28.71
ATOM	202	CB	TYR	1082	71.139	29.964	65.946	1.00	29.28
ATOM	203	CG	TYR	1082	71.171	29.063	67.161	1.00	29.31
ATOM	204	CD1	TYR	1082	70.439	27.883	67.191	1.00	32.22
ATOM	205	CE1	TYR	1082	70.458	27.048	68.308	1.00	35.00
ATOM	206	CD2	TYR	1082	71.928	29.395	68.281	1.00	29.57
ATOM	207	CE2	TYR	1082	71.957	28.570	69.406	1.00	32.16
ATOM	208	CZ	TYR	1082	71.216	27.395	69.415	1.00	34.16
ATOM	209	OH	TYR	1082	71.214	26.568	70.524	1.00	34.78
ATOM	210	C	TYR	1082	72.005	28.218	64.398	1.00	28.97
ATOM	211	O	TYR	1082	72.591	27.286	64.945	1.00	31.64
ATOM	212	N	HIS	1083	71.200	28.046	63.350	1.00	28.60
ATOM	213	CA	HIS	1083	70.943	26.717	62.800	1.00	29.08
ATOM	214	CB	HIS	1083	69.730	26.725	61.858	1.00	28.98
ATOM	215	CG	HIS	1083	69.984	27.333	60.508	1.00	27.71
ATOM	216	CD2	HIS	1083	70.696	26.886	59.443	1.00	27.80
ATOM	217	ND1	HIS	1083	69.392	28.509	60.106	1.00	26.55
ATOM	218	CE1	HIS	1083	69.724	28.766	58.852	1.00	28.23
ATOM	219	NE2	HIS	1083	70.514	27.795	58.427	1.00	28.18
ATOM	220	C	HIS	1083	72.153	26.103	62.102	1.00	31.61
ATOM	221	O	HIS	1083	72.056	25.016	61.516	1.00	32.83
ATOM	222	N	GLY	1084	73.270	26.826	62.110	1.00	31.35
ATOM	223	CA	GLY	1084	74.479	26.329	61.486	1.00	30.49
ATOM	224	C	GLY	1084	75.597	26.297	62.501	1.00	30.79
ATOM	225	O	GLY	1084	76.345	25.322	62.586	1.00	31.01
ATOM	226	N	ALA	1085	75.710	27.364	63.281	1.00	29.67
ATOM	227	CA	ALA	1085	76.756	27.463	64.291	1.00	29.18
ATOM	228	CB	ALA	1085	77.102	28.919	64.538	1.00	27.13
ATOM	229	C	ALA	1085	76.385	26.797	65.608	1.00	30.86
ATOM	230	O	ALA	1085	77.229	26.191	66.266	1.00	32.83
ATOM	231	N	GLY	1086	75.120	26.912	65.996	1.00	31.95
ATOM	232	CA	GLY	1086	74.691	26.347	67.259	1.00	30.00
ATOM	233	C	GLY	1086	75.280	27.240	68.329	1.00	30.52
ATOM	234	O	GLY	1086	75.093	28.456	68.288	1.00	31.56
ATOM	235	N	THR	1087	76.004	26.659	69.277	1.00	29.74
ATOM	236	CA	THR	1087	76.632	27.445	70.334	1.00	29.99
ATOM	237	CB	THR	1087	76.202	26.964	71.722	1.00	31.53
ATOM	238	OG1	THR	1087	76.282	25.531	71.779	1.00	33.33
ATOM	239	CG2	THR	1087	74.792	27.428	72.043	1.00	32.33
ATOM	240	C	THR	1087	78.138	27.277	70.235	1.00	29.06
ATOM	241	O	THR	1087	78.863	27.526	71.195	1.00	29.33
ATOM	242	N	ARG	1088	78.602	26.848	69.068	1.00	27.32
ATOM	243	CA	ARG	1088	80.013	26.607	68.849	1.00	25.61
ATOM	244	CB	ARG	1088	80.232	25.970	67.484	1.00	24.43
ATOM	245	CG	ARG	1088	79.894	24.510	67.450	1.00	24.44
ATOM	246	CD	ARG	1088	79.804	24.007	66.034	1.00	26.01
ATOM	247	NE	ARG	1088	78.457	23.542	65.721	1.00	25.14
ATOM	248	CZ	ARG	1088	78.181	22.324	65.274	1.00	27.41
ATOM	249	NH1	ARG	1088	79.162	21.449	65.099	1.00	29.46

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FIGURE 3 (CONT.)

ATOM	250	NH2	ARG	1088	76.937	21.999	64.942	1.00	27.99
ATOM	251	C	ARG	1088	80.880	27.837	68.974	1.00	26.13
ATOM	252	O	ARG	1088	80.407	28.963	68.843	1.00	27.98
ATOM	253	N	THR	1089	82.145	27.598	69.294	1.00	25.72
ATOM	254	CA	THR	1089	83.135	28.648	69.412	1.00	24.74
ATOM	255	CB	THR	1089	84.295	28.219	70.320	1.00	21.05
ATOM	256	OG1	THR	1089	84.682	26.880	69.991	1.00	21.01
ATOM	257	CG2	THR	1089	83.908	28.296	71.765	1.00	21.52
ATOM	258	C	THR	1089	83.699	28.785	68.012	1.00	25.12
ATOM	259	O	THR	1089	83.616	27.844	67.218	1.00	27.12
ATOM	260	N	ILE	1090	84.252	29.944	67.694	1.00	23.10
ATOM	261	CA	ILE	1090	84.854	30.135	66.392	1.00	22.50
ATOM	262	CB	ILE	1090	84.540	31.546	65.840	1.00	21.33
ATOM	263	CG2	ILE	1090	85.167	32.617	66.699	1.00	20.09
ATOM	264	CG1	ILE	1090	84.962	31.653	64.378	1.00	20.03
ATOM	265	CD1	ILE	1090	84.429	32.877	63.701	1.00	19.81
ATOM	266	C	ILE	1090	86.358	29.896	66.581	1.00	24.31
ATOM	267	O	ILE	1090	86.924	30.289	67.611	1.00	25.80
ATOM	268	N	ALA	1091	86.981	29.177	65.649	1.00	23.50
ATOM	269	CA	ALA	1091	88.412	28.883	65.728	1.00	23.75
ATOM	270	CB	ALA	1091	88.797	27.871	64.670	1.00	22.92
ATOM	271	C	ALA	1091	89.267	30.147	65.589	1.00	25.79
ATOM	272	O	ALA	1091	88.962	31.039	64.789	1.00	27.65
ATOM	273	N	SER	1092	90.354	30.201	66.349	1.00	25.22
ATOM	274	CA	SER	1092	91.271	31.335	66.345	1.00	24.64
ATOM	275	CB	SER	1092	90.898	32.264	67.501	1.00	24.34
ATOM	276	OG	SER	1092	91.981	33.043	67.962	1.00	27.32
ATOM	277	C	SER	1092	92.686	30.778	66.518	1.00	26.18
ATOM	278	O	SER	1092	92.859	29.722	67.129	1.00	28.18
ATOM	279	N	PRO	1093	93.712	31.449	65.953	1.00	26.97
ATOM	280	CD	PRO	1093	93.667	32.638	65.084	1.00	27.37
ATOM	281	CA	PRO	1093	95.094	30.955	66.092	1.00	27.58
ATOM	282	CB	PRO	1093	95.888	31.857	65.133	1.00	26.90
ATOM	283	CG	PRO	1093	95.105	33.123	65.128	1.00	28.05
ATOM	284	C	PRO	1093	95.618	31.011	67.533	1.00	27.01
ATOM	285	O	PRO	1093	96.778	30.729	67.803	1.00	25.78
ATOM	286	N	LYS	1094	94.742	31.398	68.447	1.00	28.06
ATOM	287	CA	LYS	1094	95.060	31.469	69.858	1.00	29.03
ATOM	288	CB	LYS	1094	94.935	32.901	70.355	1.00	27.19
ATOM	289	CG	LYS	1094	96.041	33.832	69.933	1.00	30.62
ATOM	290	CD	LYS	1094	95.763	35.182	70.569	1.00	34.13
ATOM	291	CE	LYS	1094	96.891	36.178	70.407	1.00	36.40
ATOM	292	NZ	LYS	1094	96.526	37.422	71.149	1.00	40.35
ATOM	293	C	LYS	1094	94.058	30.599	70.617	1.00	29.44
ATOM	294	O	LYS	1094	93.960	30.680	71.842	1.00	30.88
ATOM	295	N	GLY	1095	93.298	29.787	69.889	1.00	30.20
ATOM	296	CA	GLY	1095	92.310	28.930	70.523	1.00	30.19
ATOM	297	C	GLY	1095	90.878	29.342	70.217	1.00	29.06
ATOM	298	O	GLY	1095	90.654	30.374	69.580	1.00	28.17
ATOM	299	N	PRO	1096	89.882	28.553	70.660	1.00	28.19
ATOM	300	CD	PRO	1096	90.042	27.313	71.439	1.00	26.15

FIGURE 3 (CONT.)

ATOM	301	CA	PRO	1096	88.461	28.827	70.433	1.00	27.36
ATOM	302	CB	PRO	1096	87.780	27.625	71.083	1.00	27.13
ATOM	303	CG	PRO	1096	88.735	27.236	72.166	1.00	24.95
ATOM	304	C	PRO	1096	87.977	30.124	71.047	1.00	26.27
ATOM	305	O	PRO	1096	88.301	30.430	72.194	1.00	27.96
ATOM	306	N	VAL	1097	87.173	30.862	70.294	1.00	24.47
ATOM	307	CA	VAL	1097	86.627	32.130	70.755	1.00	24.49
ATOM	308	CB	VAL	1097	86.875	33.243	69.719	1.00	22.40
ATOM	309	CG1	VAL	1097	86.522	34.605	70.300	1.00	20.17
ATOM	310	CG2	VAL	1097	88.314	33.214	69.269	1.00	20.81
ATOM	311	C	VAL	1097	85.131	31.928	70.937	1.00	25.90
ATOM	312	O	VAL	1097	84.464	31.381	70.065	1.00	27.10
ATOM	313	N	ILE	1098	84.598	32.365	72.066	1.00	27.33
ATOM	314	CA	ILE	1098	83.182	32.179	72.326	1.00	28.53
ATOM	315	CB	ILE	1098	82.905	31.988	73.815	1.00	28.58
ATOM	316	CG2	ILE	1098	83.811	30.911	74.360	1.00	27.94
ATOM	317	CG1	ILE	1098	83.120	33.299	74.568	1.00	30.72
ATOM	318	CD1	ILE	1098	82.509	33.302	75.955	1.00	34.23
ATOM	319	C	ILE	1098	82.278	33.277	71.785	1.00	29.52
ATOM	320	O	ILE	1098	82.671	34.441	71.676	1.00	29.80
ATOM	321	N	GLN	1099	81.050	32.886	71.471	1.00	29.40
ATOM	322	CA	GLN	1099	80.064	33.804	70.933	1.00	28.62
ATOM	323	CB	GLN	1099	78.738	33.078	70.717	1.00	26.55
ATOM	324	CG	GLN	1099	78.850	31.815	69.887	1.00	23.75
ATOM	325	CD	GLN	1099	77.506	31.260	69.498	1.00	23.24
ATOM	326	OE1	GLN	1099	76.475	31.676	70.018	1.00	24.67
ATOM	327	NE2	GLN	1099	77.507	30.317	68.570	1.00	25.50
ATOM	328	C	GLN	1099	79.842	34.976	71.865	1.00	29.81
ATOM	329	O	GLN	1099	79.799	34.803	73.081	1.00	30.77
ATOM	330	N	MET	1100	79.802	36.175	71.293	1.00	30.86
ATOM	331	CA	MET	1100	79.545	37.388	72.057	1.00	31.65
ATOM	332	CB	MET	1100	79.942	38.628	71.260	1.00	33.79
ATOM	333	CG	MET	1100	81.407	38.978	71.236	1.00	36.58
ATOM	334	SD	MET	1100	81.638	40.325	70.061	1.00	40.15
ATOM	335	CE	MET	1100	81.416	41.748	71.118	1.00	41.86
ATOM	336	C	MET	1100	78.043	37.439	72.266	1.00	32.12
ATOM	337	O	MET	1100	77.565	37.967	73.266	1.00	31.59
ATOM	338	N	TYR	1101	77.305	36.926	71.281	1.00	32.79
ATOM	339	CA	TYR	1101	75.847	36.914	71.320	1.00	32.46
ATOM	340	CB	TYR	1101	75.277	38.034	70.446	1.00	31.02
ATOM	341	CG	TYR	1101	75.930	39.378	70.636	1.00	31.88
ATOM	342	CD1	TYR	1101	76.961	39.795	69.792	1.00	34.30
ATOM	343	CE1	TYR	1101	77.591	41.018	69.973	1.00	33.36
ATOM	344	CD2	TYR	1101	75.540	40.224	71.667	1.00	30.84
ATOM	345	CE2	TYR	1101	76.162	41.446	71.857	1.00	31.48
ATOM	346	CZ	TYR	1101	77.186	41.833	71.008	1.00	34.27
ATOM	347	OH	TYR	1101	77.828	43.035	71.205	1.00	40.40
ATOM	348	C	TYR	1101	75.300	35.593	70.802	1.00	33.51
ATOM	349	O	TYR	1101	75.825	35.025	69.852	1.00	32.08
ATOM	350	N	THR	1102	74.247	35.113	71.449	1.00	35.21
ATOM	351	CA	THR	1102	73.571	33.889	71.063	1.00	36.92

FIGURE 3 (CONT.)

ATOM	352	CB	THR	1102	73.904	32.722	71.996	1.00	35.96
ATOM	353	OG1	THR	1102	75.323	32.600	72.131	1.00	38.23
ATOM	354	CG2	THR	1102	73.356	31.429	71.426	1.00	37.30
ATOM	355	C	THR	1102	72.102	34.232	71.220	1.00	39.19
ATOM	356	O	THR	1102	71.663	34.661	72.292	1.00	39.17
ATOM	357	N	ASN	1103	71.351	34.079	70.140	1.00	42.34
ATOM	358	CA	ASN	1103	69.932	34.395	70.139	1.00	45.00
ATOM	359	CB	ASN	1103	69.708	35.765	69.491	1.00	47.82
ATOM	360	CG	ASN	1103	68.276	36.248	69.622	1.00	50.28
ATOM	361	OD1	ASN	1103	67.325	35.471	69.499	1.00	50.88
ATOM	362	ND2	ASN	1103	68.114	37.536	69.889	1.00	51.98
ATOM	363	C	ASN	1103	69.198	33.315	69.356	1.00	46.48
ATOM	364	O	ASN	1103	68.956	33.457	68.157	1.00	47.79
ATOM	365	N	VAL	1104	68.862	32.227	70.038	1.00	47.60
ATOM	366	CA	VAL	1104	68.170	31.115	69.407	1.00	48.19
ATOM	367	CB	VAL	1104	67.859	30.009	70.423	1.00	48.12
ATOM	368	CG1	VAL	1104	67.298	28.787	69.713	1.00	48.17
ATOM	369	CG2	VAL	1104	69.120	29.646	71.196	1.00	48.35
ATOM	370	C	VAL	1104	66.882	31.549	68.711	1.00	49.41
ATOM	371	O	VAL	1104	66.608	31.095	67.602	1.00	49.88
ATOM	372	N	ASP	1105	66.115	32.437	69.343	1.00	50.15
ATOM	373	CA	ASP	1105	64.856	32.921	68.770	1.00	51.06
ATOM	374	CB	ASP	1105	64.190	33.946	69.697	1.00	54.26
ATOM	375	CG	ASP	1105	63.123	33.329	70.588	1.00	57.62
ATOM	376	OD1	ASP	1105	62.581	34.062	71.446	1.00	59.65
ATOM	377	OD2	ASP	1105	62.819	32.125	70.428	1.00	59.74
ATOM	378	C	ASP	1105	65.023	33.537	67.394	1.00	50.07
ATOM	379	O	ASP	1105	64.264	33.238	66.467	1.00	52.01
ATOM	380	N	GLN	1106	66.022	34.397	67.262	1.00	47.71
ATOM	381	CA	GLN	1106	66.276	35.061	65.997	1.00	45.61
ATOM	382	CB	GLN	1106	66.844	36.452	66.252	1.00	47.45
ATOM	383	CG	GLN	1106	65.850	37.347	66.976	1.00	52.29
ATOM	384	CD	GLN	1106	66.365	38.750	67.222	1.00	54.66
ATOM	385	OE1	GLN	1106	67.565	38.964	67.405	1.00	56.39
ATOM	386	NE2	GLN	1106	65.455	39.719	67.233	1.00	54.76
ATOM	387	C	GLN	1106	67.161	34.281	65.034	1.00	43.29
ATOM	388	O	GLN	1106	67.370	34.715	63.904	1.00	44.19
ATOM	389	N	ASP	1107	67.629	33.110	65.458	1.00	40.90
ATOM	390	CA	ASP	1107	68.503	32.279	64.630	1.00	39.02
ATOM	391	CB	ASP	1107	67.818	31.993	63.288	1.00	36.53
ATOM	392	CG	ASP	1107	68.386	30.779	62.580	1.00	38.24
ATOM	393	OD1	ASP	1107	69.035	29.937	63.233	1.00	39.97
ATOM	394	OD2	ASP	1107	68.156	30.655	61.363	1.00	39.42
ATOM	395	C	ASP	1107	69.813	33.045	64.407	1.00	38.47
ATOM	396	O	ASP	1107	70.500	32.848	63.406	1.00	38.85
ATOM	397	N	LEU	1108	70.192	33.845	65.400	1.00	37.86
ATOM	398	CA	LEU	1108	71.369	34.702	65.316	1.00	37.42
ATOM	399	CB	LEU	1108	70.901	36.155	65.431	1.00	35.72
ATOM	400	CG	LEU	1108	71.902	37.299	65.315	1.00	33.41
ATOM	401	CD1	LEU	1108	72.538	37.304	63.944	1.00	33.86
ATOM	402	CD2	LEU	1108	71.163	38.594	65.539	1.00	35.77

FIGURE 3 (CONT.)

ATOM	403	C	LEU	1108	72.445	34.471	66.366	1.00	37.37
ATOM	404	O	LEU	1108	72.145	34.391	67.558	1.00	38.07
ATOM	405	N	VAL	1109	73.698	34.388	65.924	1.00	35.09
ATOM	406	CA	VAL	1109	74.830	34.228	66.838	1.00	33.17
ATOM	407	CB	VAL	1109	75.296	32.744	67.025	1.00	32.32
ATOM	408	CG1	VAL	1109	74.117	31.841	67.272	1.00	32.33
ATOM	409	CG2	VAL	1109	76.119	32.264	65.860	1.00	31.84
ATOM	410	C	VAL	1109	75.972	35.070	66.296	1.00	31.38
ATOM	411	O	VAL	1109	76.080	35.272	65.087	1.00	32.93
ATOM	412	N	GLY	1110	76.815	35.570	67.183	1.00	29.70
ATOM	413	CA	GLY	1110	77.917	36.394	66.743	1.00	26.58
ATOM	414	C	GLY	1110	79.129	36.273	67.627	1.00	25.55
ATOM	415	O	GLY	1110	79.008	36.097	68.840	1.00	25.57
ATOM	416	N	TRP	1111	80.300	36.317	67.004	1.00	24.66
ATOM	417	CA	TRP	1111	81.574	36.241	67.713	1.00	23.97
ATOM	418	CB	TRP	1111	82.415	35.077	67.186	1.00	22.57
ATOM	419	CG	TRP	1111	81.754	33.720	67.136	1.00	22.78
ATOM	420	CD2	TRP	1111	81.163	33.091	65.987	1.00	20.85
ATOM	421	CE2	TRP	1111	80.824	31.772	66.360	1.00	19.39
ATOM	422	CE3	TRP	1111	80.906	33.510	64.674	1.00	18.90
ATOM	423	CD1	TRP	1111	81.725	32.785	68.135	1.00	21.78
ATOM	424	NE1	TRP	1111	81.175	31.614	67.675	1.00	21.65
ATOM	425	CZ2	TRP	1111	80.240	30.870	65.474	1.00	19.81
ATOM	426	CZ3	TRP	1111	80.324	32.613	63.790	1.00	18.79
ATOM	427	CH2	TRP	1111	80.001	31.306	64.193	1.00	20.56
ATOM	428	C	TRP	1111	82.298	37.532	67.355	1.00	25.16
ATOM	429	O	TRP	1111	81.788	38.321	66.563	1.00	25.20
ATOM	430	N	PRO	1112	83.451	37.813	67.989	1.00	25.84
ATOM	431	CD	PRO	1112	84.090	37.167	69.149	1.00	25.27
ATOM	432	CA	PRO	1112	84.159	39.048	67.627	1.00	24.42
ATOM	433	CB	PRO	1112	85.322	39.063	68.611	1.00	23.55
ATOM	434	CG	PRO	1112	84.768	38.329	69.801	1.00	23.65
ATOM	435	C	PRO	1112	84.666	38.826	66.194	1.00	25.76
ATOM	436	O	PRO	1112	84.988	37.693	65.829	1.00	27.02
ATOM	437	N	ALA	1113	84.697	39.863	65.366	1.00	23.75
ATOM	438	CA	ALA	1113	85.159	39.686	63.995	1.00	22.81
ATOM	439	CB	ALA	1113	85.051	40.980	63.239	1.00	25.86
ATOM	440	C	ALA	1113	86.592	39.158	63.959	1.00	23.10
ATOM	441	O	ALA	1113	87.491	39.730	64.567	1.00	25.15
ATOM	442	N	PRO	1114	86.826	38.071	63.212	1.00	23.57
ATOM	443	CD	PRO	1114	85.827	37.384	62.375	1.00	24.85
ATOM	444	CA	PRO	1114	88.135	37.433	63.074	1.00	24.09
ATOM	445	CB	PRO	1114	87.790	36.144	62.340	1.00	23.05
ATOM	446	CG	PRO	1114	86.691	36.587	61.430	1.00	23.55
ATOM	447	C	PRO	1114	89.160	38.250	62.296	1.00	27.35
ATOM	448	O	PRO	1114	88.904	39.390	61.896	1.00	28.70
ATOM	449	N	GLN	1115	90.324	37.654	62.078	1.00	28.98
ATOM	450	CA	GLN	1115	91.380	38.312	61.331	1.00	32.07
ATOM	451	CB	GLN	1115	92.747	37.751	61.726	1.00	35.02
ATOM	452	CG	GLN	1115	93.188	38.161	63.107	1.00	40.55
ATOM	453	CD	GLN	1115	94.606	37.721	63.422	1.00	43.24

FIGURE 3 (CONT.)

ATOM	454	OE1	GLN	1115	94.851	36.571	63.793	1.00	41.11
ATOM	455	NE2	GLN	1115	95.547	38.649	63.308	1.00	45.52
ATOM	456	C	GLN	1115	91.168	38.171	59.821	1.00	31.93
ATOM	457	O	GLN	1115	90.705	37.137	59.329	1.00	30.69
ATOM	458	N	GLY	1116	91.512	39.225	59.093	1.00	31.14
ATOM	459	CA	GLY	1116	91.354	39.206	57.653	1.00	29.19
ATOM	460	C	GLY	1116	89.973	39.686	57.271	1.00	27.79
ATOM	461	O	GLY	1116	89.578	39.579	56.109	1.00	28.10
ATOM	462	N	SER	1117	89.249	40.247	58.237	1.00	25.03
ATOM	463	CA	SER	1117	87.909	40.729	57.973	1.00	24.84
ATOM	464	CB	SER	1117	86.904	40.042	58.899	1.00	23.52
ATOM	465	OG	SER	1117	86.986	40.560	60.214	1.00	21.42
ATOM	466	C	SER	1117	87.800	42.226	58.161	1.00	25.97
ATOM	467	O	SER	1117	88.671	42.846	58.768	1.00	27.89
ATOM	468	N	ARG	1118	86.742	42.796	57.591	1.00	26.62
ATOM	469	CA	ARG	1118	86.416	44.208	57.719	1.00	25.45
ATOM	470	CB	ARG	1118	86.940	45.048	56.545	1.00	28.49
ATOM	471	CG	ARG	1118	86.095	45.116	55.292	1.00	32.87
ATOM	472	CD	ARG	1118	86.240	46.504	54.632	1.00	40.52
ATOM	473	NE	ARG	1118	85.263	47.482	55.135	1.00	46.91
ATOM	474	CZ	ARG	1118	84.084	47.729	54.558	1.00	48.20
ATOM	475	NH1	ARG	1118	83.741	47.085	53.444	1.00	49.22
ATOM	476	NH2	ARG	1118	83.217	48.567	55.114	1.00	50.55
ATOM	477	C	ARG	1118	84.894	44.224	57.812	1.00	24.87
ATOM	478	O	ARG	1118	84.224	43.400	57.192	1.00	23.66
ATOM	479	N	SER	1119	84.354	45.088	58.659	1.00	24.12
ATOM	480	CA	SER	1119	82.917	45.142	58.848	1.00	21.38
ATOM	481	CB	SER	1119	82.566	45.698	60.221	1.00	19.53
ATOM	482	OG	SER	1119	82.806	44.732	61.235	1.00	18.13
ATOM	483	C	SER	1119	82.134	45.881	57.789	1.00	22.88
ATOM	484	O	SER	1119	82.661	46.738	57.076	1.00	22.56
ATOM	485	N	LEU	1120	80.872	45.486	57.682	1.00	23.25
ATOM	486	CA	LEU	1120	79.915	46.057	56.758	1.00	24.37
ATOM	487	CB	LEU	1120	78.950	44.979	56.290	1.00	23.76
ATOM	488	CG	LEU	1120	78.911	44.542	54.840	1.00	23.49
ATOM	489	CD1	LEU	1120	77.753	43.571	54.701	1.00	21.66
ATOM	490	CD2	LEU	1120	78.726	45.752	53.934	1.00	22.71
ATOM	491	C	LEU	1120	79.107	47.107	57.510	1.00	27.32
ATOM	492	O	LEU	1120	78.891	46.994	58.725	1.00	28.09
ATOM	493	N	THR	1121	78.618	48.096	56.771	1.00	30.14
ATOM	494	CA	THR	1121	77.821	49.176	57.334	1.00	29.30
ATOM	495	CB	THR	1121	78.065	50.474	56.574	1.00	29.90
ATOM	496	OG1	THR	1121	79.457	50.575	56.236	1.00	32.57
ATOM	497	CG2	THR	1121	77.650	51.656	57.415	1.00	28.80
ATOM	498	C	THR	1121	76.361	48.835	57.150	1.00	30.05
ATOM	499	O	THR	1121	75.955	48.396	56.075	1.00	32.34
ATOM	500	N	PRO	1122	75.546	49.021	58.190	1.00	29.89
ATOM	501	CD	PRO	1122	75.910	49.352	59.571	1.00	29.08
ATOM	502	CA	PRO	1122	74.118	48.717	58.088	1.00	29.25
ATOM	503	CB	PRO	1122	73.637	48.907	59.517	1.00	28.58
ATOM	504	CG	PRO	1122	74.856	48.613	60.323	1.00	30.38

ATOM	505	C	PRO	1122	73.427	49.703	57.145	1.00	30.47
ATOM	506	O	PRO	1122	73.874	50.839	56.986	1.00	32.91
ATOM	507	N	CYS	1123	72.346	49.271	56.511	1.00	30.63
ATOM	508	CA	CYS	1123	71.621	50.136	55.596	1.00	30.60
ATOM	509	CB	CYS	1123	70.614	49.332	54.778	1.00	29.72
ATOM	510	SG	CYS	1123	69.790	50.297	53.488	1.00	25.00
ATOM	511	C	CYS	1123	70.906	51.235	56.384	1.00	32.65
ATOM	512	O	CYS	1123	70.541	51.047	57.546	1.00	31.99
ATOM	513	N	THR	1124	70.744	52.393	55.755	1.00	34.65
ATOM	514	CA	THR	1124	70.082	53.533	56.377	1.00	36.02
ATOM	515	CB	THR	1124	71.118	54.557	56.908	1.00	36.13
ATOM	516	OG1	THR	1124	71.877	55.082	55.810	1.00	36.33
ATOM	517	CG2	THR	1124	72.074	53.903	57.908	1.00	34.16
ATOM	518	C	THR	1124	69.208	54.236	55.337	1.00	37.69
ATOM	519	O	THR	1124	68.718	55.341	55.576	1.00	40.17
ATOM	520	N	CYS	1125	69.040	53.609	54.174	1.00	37.56
ATOM	521	CA	CYS	1125	68.243	54.202	53.110	1.00	35.40
ATOM	522	CB	CYS	1125	69.001	54.161	51.775	1.00	36.85
ATOM	523	SG	CYS	1125	69.270	52.512	51.083	1.00	37.80
ATOM	524	C	CYS	1125	66.884	53.548	52.958	1.00	34.49
ATOM	525	O	CYS	1125	66.079	53.974	52.139	1.00	36.12
ATOM	526	N	GLY	1126	66.637	52.496	53.725	1.00	34.32
ATOM	527	CA	GLY	1126	65.358	51.813	53.650	1.00	33.36
ATOM	528	C	GLY	1126	64.953	51.332	52.271	1.00	32.12
ATOM	529	O	GLY	1126	63.764	51.212	51.976	1.00	33.53
ATOM	530	N	SER	1127	65.931	51.066	51.417	1.00	30.17
ATOM	531	CA	SER	1127	65.636	50.584	50.082	1.00	30.11
ATOM	532	CB	SER	1127	66.886	50.595	49.220	1.00	30.14
ATOM	533	OG	SER	1127	66.565	50.233	47.893	1.00	31.03
ATOM	534	C	SER	1127	65.090	49.165	50.154	1.00	31.51
ATOM	535	O	SER	1127	65.455	48.392	51.042	1.00	33.06
ATOM	536	N	SER	1128	64.232	48.823	49.201	1.00	32.01
ATOM	537	CA	SER	1128	63.625	47.501	49.140	1.00	32.06
ATOM	538	CB	SER	1128	62.125	47.633	48.916	1.00	33.84
ATOM	539	OG	SER	1128	61.868	48.596	47.908	1.00	39.40
ATOM	540	C	SER	1128	64.246	46.652	48.042	1.00	31.04
ATOM	541	O	SER	1128	63.892	45.490	47.866	1.00	30.15
ATOM	542	N	ASP	1129	65.153	47.244	47.281	1.00	31.57
ATOM	543	CA	ASP	1129	65.838	46.521	46.221	1.00	30.82
ATOM	544	CB	ASP	1129	66.170	47.478	45.071	1.00	32.94
ATOM	545	CG	ASP	1129	64.925	48.168	44.512	1.00	37.09
ATOM	546	OD1	ASP	1129	64.087	47.488	43.876	1.00	38.85
ATOM	547	OD2	ASP	1129	64.769	49.388	44.731	1.00	40.93
ATOM	548	C	ASP	1129	67.101	45.931	46.838	1.00	28.43
ATOM	549	O	ASP	1129	68.110	46.617	46.966	1.00	28.53
ATOM	550	N	LEU	1130	67.006	44.679	47.280	1.00	28.60
ATOM	551	CA	LEU	1130	68.114	43.965	47.922	1.00	27.20
ATOM	552	CB	LEU	1130	67.570	43.060	49.026	1.00	25.89
ATOM	553	CG	LEU	1130	66.449	43.614	49.910	1.00	27.61
ATOM	554	CD1	LEU	1130	66.230	42.644	51.049	1.00	30.67
ATOM	555	CD2	LEU	1130	66.781	44.991	50.455	1.00	26.86

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FIGURE 8 (CONT.)

ATOM	556	C	LEU	1130	68.955	43.122	46.955	1.00	27.30
ATOM	557	O	LEU	1130	68.524	42.812	45.847	1.00	29.26
ATOM	558	N	TYR	1131	70.155	42.740	47.386	1.00	26.38
ATOM	559	CA	TYR	1131	71.060	41.939	46.572	1.00	24.28
ATOM	560	CB	TYR	1131	72.118	42.830	45.922	1.00	22.21
ATOM	561	CG	TYR	1131	71.528	43.904	45.044	1.00	23.22
ATOM	562	CD1	TYR	1131	71.208	45.151	45.562	1.00	23.25
ATOM	563	CE1	TYR	1131	70.601	46.129	44.772	1.00	25.08
ATOM	564	CD2	TYR	1131	71.234	43.654	43.707	1.00	24.48
ATOM	565	CE2	TYR	1131	70.626	44.627	42.905	1.00	24.25
ATOM	566	CZ	TYR	1131	70.311	45.860	43.447	1.00	25.18
ATOM	567	OH	TYR	1131	69.697	46.824	42.673	1.00	26.26
ATOM	568	C	TYR	1131	71.725	40.924	47.479	1.00	24.97
ATOM	569	O	TYR	1131	72.462	41.293	48.386	1.00	27.58
ATOM	570	N	LEU	1132	71.431	39.649	47.259	1.00	24.30
ATOM	571	CA	LEU	1132	71.984	38.569	48.067	1.00	24.74
ATOM	572	CB	LEU	1132	70.964	37.438	48.186	1.00	24.61
ATOM	573	CG	LEU	1132	71.334	36.245	49.064	1.00	22.52
ATOM	574	CD1	LEU	1132	70.194	36.009	50.007	1.00	27.96
ATOM	575	CD2	LEU	1132	71.605	35.009	48.230	1.00	23.92
ATOM	576	C	LEU	1132	73.276	38.023	47.489	1.00	25.14
ATOM	577	O	LEU	1132	73.350	37.746	46.297	1.00	27.15
ATOM	578	N	VAL	1133	74.288	37.857	48.333	1.00	25.08
ATOM	579	CA	VAL	1133	75.577	37.327	47.890	1.00	24.16
ATOM	580	CB	VAL	1133	76.757	38.156	48.445	1.00	23.60
ATOM	581	CG1	VAL	1133	78.076	37.629	47.872	1.00	19.70
ATOM	582	CG2	VAL	1133	76.556	39.645	48.134	1.00	18.12
ATOM	583	C	VAL	1133	75.719	35.890	48.377	1.00	24.92
ATOM	584	O	VAL	1133	75.573	35.620	49.572	1.00	25.15
ATOM	585	N	THR	1134	75.987	34.969	47.456	1.00	24.88
ATOM	586	CA	THR	1134	76.125	33.563	47.812	1.00	25.34
ATOM	587	CB	THR	1134	75.611	32.638	46.677	1.00	27.21
ATOM	588	OG1	THR	1134	76.498	32.698	45.550	1.00	26.50
ATOM	589	CG2	THR	1134	74.204	33.054	46.236	1.00	24.71
ATOM	590	C	THR	1134	77.566	33.205	48.150	1.00	25.73
ATOM	591	O	THR	1134	78.476	34.010	47.944	1.00	26.83
ATOM	592	N	ARG	1135	77.776	31.981	48.630	1.00	25.40
ATOM	593	CA	ARG	1135	79.112	31.504	48.991	1.00	23.76
ATOM	594	CB	ARG	1135	79.027	30.150	49.689	1.00	22.71
ATOM	595	CG	ARG	1135	78.413	29.062	48.835	1.00	25.45
ATOM	596	CD	ARG	1135	78.383	27.742	49.566	1.00	26.50
ATOM	597	NE	ARG	1135	79.722	27.265	49.897	1.00	27.92
ATOM	598	CZ	ARG	1135	80.174	27.097	51.135	1.00	27.79
ATOM	599	NH1	ARG	1135	79.405	27.366	52.180	1.00	28.04
ATOM	600	NH2	ARG	1135	81.404	26.652	51.327	1.00	30.59
ATOM	601	C	ARG	1135	80.038	31.382	47.792	1.00	24.58
ATOM	602	O	ARG	1135	81.219	31.091	47.950	1.00	25.10
ATOM	603	N	HIS	1136	79.496	31.546	46.589	1.00	25.35
ATOM	604	CA	HIS	1136	80.303	31.451	45.378	1.00	26.27
ATOM	605	CB	HIS	1136	79.618	30.551	44.348	1.00	26.38
ATOM	606	CG	HIS	1136	79.283	29.194	44.872	1.00	27.82

FIGURE 3 (CONT.)

ATOM	607	CD2	HIS	1136	78.091	28.629	45.174	1.00	28.51
ATOM	608	ND1	HIS	1136	80.242	28.264	45.213	1.00	29.89
ATOM	609	CE1	HIS	1136	79.657	27.188	45.710	1.00	29.44
ATOM	610	NE2	HIS	1136	78.353	27.387	45.697	1.00	31.77
ATOM	611	C	HIS	1136	80.540	32.834	44.794	1.00	26.66
ATOM	612	O	HIS	1136	81.064	32.966	43.686	1.00	27.04
ATOM	613	N	ALA	1137	80.126	33.850	45.552	1.00	26.65
ATOM	614	CA	ALA	1137	80.265	35.253	45.179	1.00	25.32
ATOM	615	CB	ALA	1137	81.675	35.532	44.664	1.00	26.21
ATOM	616	C	ALA	1137	79.219	35.743	44.177	1.00	25.87
ATOM	617	O	ALA	1137	79.280	36.890	43.724	1.00	24.80
ATOM	618	N	ASP	1138	78.256	34.887	43.837	1.00	24.81
ATOM	619	CA	ASP	1138	77.203	35.277	42.903	1.00	23.77
ATOM	620	CB	ASP	1138	76.301	34.091	42.536	1.00	26.17
ATOM	621	CG	ASP	1138	77.038	32.962	41.827	1.00	27.49
ATOM	622	OD1	ASP	1138	77.712	33.214	40.807	1.00	27.61
ATOM	623	OD2	ASP	1138	76.891	31.801	42.268	1.00	28.37
ATOM	624	C	ASP	1138	76.344	36.301	43.629	1.00	22.53
ATOM	625	O	ASP	1138	76.282	36.302	44.856	1.00	23.66
ATOM	626	N	VAL	1139	75.699	37.180	42.881	1.00	21.63
ATOM	627	CA	VAL	1139	74.828	38.178	43.477	1.00	22.35
ATOM	628	CB	VAL	1139	75.287	39.627	43.161	1.00	20.65
ATOM	629	CG1	VAL	1139	74.385	40.625	43.854	1.00	17.61
ATOM	630	CG2	VAL	1139	76.736	39.841	43.607	1.00	16.25
ATOM	631	C	VAL	1139	73.438	37.908	42.915	1.00	24.89
ATOM	632	O	VAL	1139	73.270	37.696	41.706	1.00	27.94
ATOM	633	N	ILE	1140	72.447	37.895	43.796	1.00	24.15
ATOM	634	CA	ILE	1140	71.071	37.606	43.425	1.00	21.78
ATOM	635	CB	ILE	1140	70.588	36.338	44.156	1.00	19.13
ATOM	636	CG2	ILE	1140	69.104	36.166	43.999	1.00	19.57
ATOM	637	CG1	ILE	1140	71.329	35.104	43.647	1.00	17.97
ATOM	638	CD1	ILE	1140	71.069	33.877	44.498	1.00	16.36
ATOM	639	C	ILE	1140	70.149	38.748	43.816	1.00	22.53
ATOM	640	O	ILE	1140	69.979	39.038	44.995	1.00	23.66
ATOM	641	N	PRO	1141	69.546	39.422	42.832	1.00	23.25
ATOM	642	CD	PRO	1141	69.768	39.320	41.383	1.00	22.90
ATOM	643	CA	PRO	1141	68.638	40.530	43.144	1.00	23.97
ATOM	644	CB	PRO	1141	68.328	41.111	41.770	1.00	24.50
ATOM	645	CG	PRO	1141	69.549	40.730	40.952	1.00	24.13
ATOM	646	C	PRO	1141	67.372	40.003	43.835	1.00	26.14
ATOM	647	O	PRO	1141	66.692	39.095	43.341	1.00	27.20
ATOM	648	N	VAL	1142	67.085	40.556	44.999	1.00	26.19
ATOM	649	CA	VAL	1142	65.936	40.161	45.788	1.00	27.02
ATOM	650	CB	VAL	1142	66.406	39.499	47.096	1.00	25.62
ATOM	651	CG1	VAL	1142	65.263	39.348	48.074	1.00	24.17
ATOM	652	CG2	VAL	1142	67.036	38.155	46.787	1.00	24.42
ATOM	653	C	VAL	1142	65.136	41.422	46.087	1.00	29.57
ATOM	654	O	VAL	1142	65.703	42.462	46.413	1.00	30.26
ATOM	655	N	ARG	1143	63.827	41.358	45.896	1.00	31.86
ATOM	656	CA	ARG	1143	62.989	42.512	46.166	1.00	35.28
ATOM	657	CB	ARG	1143	61.964	42.715	45.053	1.00	38.62

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FIGURE 3 (CONT.)

ATOM	658	CG	ARG	1143	61.555	44.152	44.880	1.00	40.15
ATOM	659	CD	ARG	1143	60.377	44.489	45.748	1.00	44.51
ATOM	660	NE	ARG	1143	60.308	45.904	46.106	1.00	51.14
ATOM	661	CZ	ARG	1143	60.485	46.926	45.269	1.00	55.15
ATOM	662	NH1	ARG	1143	60.759	46.731	43.983	1.00	57.46
ATOM	663	NH2	ARG	1143	60.355	48.166	45.723	1.00	57.00
ATOM	664	C	ARG	1143	62.316	42.243	47.497	1.00	36.53
ATOM	665	O	ARG	1143	61.696	41.197	47.695	1.00	39.63
ATOM	666	N	ARG	1144	62.474	43.171	48.425	1.00	36.31
ATOM	667	CA	ARG	1144	61.917	43.010	49.750	1.00	36.40
ATOM	668	CB	ARG	1144	62.448	44.090	50.673	1.00	35.36
ATOM	669	CG	ARG	1144	62.311	43.749	52.125	1.00	35.23
ATOM	670	CD	ARG	1144	62.817	44.882	52.953	1.00	36.19
ATOM	671	NE	ARG	1144	62.992	44.497	54.346	1.00	39.02
ATOM	672	CZ	ARG	1144	63.660	45.233	55.223	1.00	40.02
ATOM	673	NH1	ARG	1144	63.786	44.834	56.481	1.00	38.46
ATOM	674	NH2	ARG	1144	64.205	46.377	54.831	1.00	42.18
ATOM	675	C	ARG	1144	60.405	43.041	49.742	1.00	38.06
ATOM	676	O	ARG	1144	59.784	43.800	48.995	1.00	37.65
ATOM	677	N	ARG	1145	59.820	42.193	50.575	1.00	40.25
ATOM	678	CA	ARG	1145	58.377	42.107	50.689	1.00	41.89
ATOM	679	CB	ARG	1145	57.897	40.717	50.278	1.00	40.89
ATOM	680	CG	ARG	1145	58.127	40.425	48.805	1.00	40.67
ATOM	681	CD	ARG	1145	57.432	41.454	47.960	1.00	40.17
ATOM	682	NE	ARG	1145	57.599	41.235	46.530	1.00	41.36
ATOM	683	CZ	ARG	1145	57.295	42.146	45.612	1.00	45.08
ATOM	684	NH1	ARG	1145	56.814	43.332	45.982	1.00	47.79
ATOM	685	NH2	ARG	1145	57.465	41.878	44.324	1.00	45.53
ATOM	686	C	ARG	1145	57.903	42.458	52.090	1.00	42.89
ATOM	687	O	ARG	1145	56.720	42.725	52.295	1.00	44.14
ATOM	688	N	GLY	1146	58.832	42.493	53.043	1.00	43.96
ATOM	689	CA	GLY	1146	58.483	42.832	54.412	1.00	44.02
ATOM	690	C	GLY	1146	59.699	42.813	55.312	1.00	43.54
ATOM	691	O	GLY	1146	60.795	42.495	54.847	1.00	44.52
ATOM	692	N	ASP	1147	59.499	43.110	56.595	1.00	42.52
ATOM	693	CA	ASP	1147	60.570	43.134	57.596	1.00	40.57
ATOM	694	CB	ASP	1147	59.987	43.005	59.013	1.00	45.28
ATOM	695	CG	ASP	1147	59.051	44.151	59.382	1.00	51.16
ATOM	696	OD1	ASP	1147	58.092	43.897	60.151	1.00	53.15
ATOM	697	OD2	ASP	1147	59.271	45.296	58.916	1.00	54.39
ATOM	698	C	ASP	1147	61.665	42.080	57.424	1.00	37.05
ATOM	699	O	ASP	1147	62.845	42.387	57.552	1.00	37.14
ATOM	700	N	SER	1148	61.283	40.840	57.150	1.00	32.32
ATOM	701	CA	SER	1148	62.278	39.794	56.996	1.00	30.82
ATOM	702	CB	SER	1148	62.436	39.055	58.321	1.00	32.46
ATOM	703	OG	SER	1148	61.246	38.376	58.667	1.00	35.71
ATOM	704	C	SER	1148	62.013	38.801	55.866	1.00	28.99
ATOM	705	O	SER	1148	62.313	37.619	56.003	1.00	26.58
ATOM	706	N	ARG	1149	61.504	39.288	54.736	1.00	29.34
ATOM	707	CA	ARG	1149	61.211	38.426	53.589	1.00	30.00
ATOM	708	CB	ARG	1149	59.760	37.914	53.663	1.00	33.43

FIGURE 3 (CONT.)

ATOM	709	CG	ARG	1149	59.363	36.826	52.655	1.00	36.36
ATOM	710	CD	ARG	1149	58.733	37.418	51.389	1.00	42.94
ATOM	711	NE	ARG	1149	57.958	36.444	50.610	1.00	46.67
ATOM	712	CZ	ARG	1149	57.764	36.514	49.291	1.00	46.83
ATOM	713	NH1	ARG	1149	58.288	37.506	48.594	1.00	45.95
ATOM	714	NH2	ARG	1149	57.021	35.603	48.668	1.00	47.58
ATOM	715	C	ARG	1149	61.442	39.191	52.290	1.00	28.92
ATOM	716	O	ARG	1149	61.181	40.401	52.206	1.00	27.96
ATOM	717	N	GLY	1150	61.921	38.471	51.282	1.00	27.08
ATOM	718	CA	GLY	1150	62.190	39.065	49.986	1.00	25.77
ATOM	719	C	GLY	1150	61.983	38.029	48.900	1.00	25.52
ATOM	720	O	GLY	1150	62.093	36.831	49.147	1.00	24.50
ATOM	721	N	SER	1151	61.672	38.479	47.694	1.00	25.63
ATOM	722	CA	SER	1151	61.441	37.572	46.583	1.00	27.27
ATOM	723	CB	SER	1151	60.076	37.859	45.960	1.00	29.08
ATOM	724	OG	SER	1151	59.833	39.257	45.883	1.00	29.83
ATOM	725	C	SER	1151	62.528	37.718	45.533	1.00	27.69
ATOM	726	O	SER	1151	62.885	38.837	45.150	1.00	28.46
ATOM	727	N	LEU	1152	63.093	36.592	45.109	1.00	26.82
ATOM	728	CA	LEU	1152	64.129	36.609	44.089	1.00	27.90
ATOM	729	CB	LEU	1152	64.658	35.202	43.828	1.00	24.63
ATOM	730	CG	LEU	1152	65.784	34.643	44.686	1.00	23.94
ATOM	731	CD1	LEU	1152	65.377	34.577	46.139	1.00	22.37
ATOM	732	CD2	LEU	1152	66.145	33.273	44.155	1.00	19.80
ATOM	733	C	LEU	1152	63.501	37.127	42.811	1.00	29.83
ATOM	734	O	LEU	1152	62.394	36.722	42.463	1.00	33.35
ATOM	735	N	LEU	1153	64.199	38.009	42.107	1.00	30.33
ATOM	736	CA	LEU	1153	63.676	38.538	40.858	1.00	29.78
ATOM	737	CB	LEU	1153	64.521	39.716	40.379	1.00	26.59
ATOM	738	CG	LEU	1153	64.020	41.065	40.896	1.00	25.76
ATOM	739	CD1	LEU	1153	63.897	41.039	42.394	1.00	24.26
ATOM	740	CD2	LEU	1153	64.940	42.176	40.444	1.00	26.30
ATOM	741	C	LEU	1153	63.643	37.433	39.808	1.00	31.23
ATOM	742	O	LEU	1153	62.853	37.474	38.869	1.00	33.74
ATOM	743	N	SER	1154	64.503	36.440	39.987	1.00	32.78
ATOM	744	CA	SER	1154	64.596	35.309	39.081	1.00	34.85
ATOM	745	CB	SER	1154	65.780	35.481	38.132	1.00	36.29
ATOM	746	OG	SER	1154	65.855	36.805	37.636	1.00	43.91
ATOM	747	C	SER	1154	64.846	34.107	39.961	1.00	35.31
ATOM	748	O	SER	1154	65.943	33.949	40.505	1.00	37.17
ATOM	749	N	PRO	1155	63.807	33.291	40.190	1.00	35.71
ATOM	750	CD	PRO	1155	62.401	33.474	39.780	1.00	36.01
ATOM	751	CA	PRO	1155	63.949	32.101	41.031	1.00	34.86
ATOM	752	CB	PRO	1155	62.599	31.419	40.871	1.00	35.84
ATOM	753	CG	PRO	1155	61.670	32.598	40.777	1.00	36.09
ATOM	754	C	PRO	1155	65.101	31.245	40.540	1.00	33.69
ATOM	755	O	PRO	1155	65.426	31.254	39.352	1.00	33.22
ATOM	756	N	ARG	1156	65.726	30.525	41.459	1.00	33.17
ATOM	757	CA	ARG	1156	66.873	29.700	41.124	1.00	35.02
ATOM	758	CB	ARG	1156	68.173	30.405	41.566	1.00	37.90
ATOM	759	CG	ARG	1156	68.856	31.265	40.505	1.00	40.72

ATOM	760	CD	ARG	1156	68.739	32.740	40.813	1.00	43.82
ATOM	761	NE	ARG	1156	69.536	33.543	39.886	1.00	49.55
ATOM	762	CZ	ARG	1156	69.696	34.864	39.972	1.00	51.56
ATOM	763	NH1	ARG	1156	69.117	35.551	40.943	1.00	52.24
ATOM	764	NH2	ARG	1156	70.452	35.502	39.089	1.00	53.76
ATOM	765	C	ARG	1156	66.799	28.348	41.804	1.00	34.39
ATOM	766	O	ARG	1156	66.115	28.193	42.811	1.00	35.64
ATOM	767	N	PRO	1157	67.501	27.344	41.258	1.00	34.78
ATOM	768	CD	PRO	1157	68.361	27.376	40.063	1.00	36.56
ATOM	769	CA	PRO	1157	67.495	26.008	41.859	1.00	35.76
ATOM	770	CB	PRO	1157	68.577	25.277	41.066	1.00	35.08
ATOM	771	CG	PRO	1157	68.488	25.916	39.721	1.00	36.87
ATOM	772	C	PRO	1157	67.930	26.189	43.305	1.00	36.38
ATOM	773	O	PRO	1157	68.824	26.993	43.579	1.00	38.01
ATOM	774	N	ILE	1158	67.317	25.456	44.226	1.00	35.10
ATOM	775	CA	ILE	1158	67.675	25.599	45.629	1.00	33.87
ATOM	776	CB	ILE	1158	66.917	24.586	46.526	1.00	33.81
ATOM	777	CG2	ILE	1158	67.042	23.174	45.973	1.00	34.22
ATOM	778	CG1	ILE	1158	67.418	24.690	47.972	1.00	36.64
ATOM	779	CD1	ILE	1158	66.985	23.541	48.876	1.00	38.94
ATOM	780	C	ILE	1158	69.185	25.486	45.834	1.00	32.49
ATOM	781	O	ILE	1158	69.765	26.236	46.610	1.00	32.56
ATOM	782	N	SER	1159	69.830	24.609	45.075	1.00	32.75
ATOM	783	CA	SER	1159	71.271	24.418	45.203	1.00	33.76
ATOM	784	CB	SER	1159	71.769	23.392	44.188	1.00	33.12
ATOM	785	OG	SER	1159	71.450	23.816	42.875	1.00	38.29
ATOM	786	C	SER	1159	72.035	25.722	45.028	1.00	32.08
ATOM	787	O	SER	1159	73.003	25.971	45.737	1.00	31.63
ATOM	788	N	TYR	1160	71.591	26.554	44.092	1.00	29.65
ATOM	789	CA	TYR	1160	72.255	27.822	43.835	1.00	27.91
ATOM	790	CB	TYR	1160	71.482	28.628	42.798	1.00	23.87
ATOM	791	CG	TYR	1160	72.293	29.740	42.158	1.00	22.81
ATOM	792	CD1	TYR	1160	73.402	29.455	41.368	1.00	22.72
ATOM	793	CE1	TYR	1160	74.132	30.476	40.755	1.00	23.32
ATOM	794	CD2	TYR	1160	71.934	31.078	42.319	1.00	23.14
ATOM	795	CE2	TYR	1160	72.656	32.104	41.704	1.00	21.74
ATOM	796	CZ	TYR	1160	73.749	31.793	40.928	1.00	22.91
ATOM	797	OH	TYR	1160	74.454	32.793	40.307	1.00	24.05
ATOM	798	C	TYR	1160	72.413	28.638	45.118	1.00	29.71
ATOM	799	O	TYR	1160	73.381	29.400	45.258	1.00	32.87
ATOM	800	N	LEU	1161	71.479	28.469	46.054	1.00	27.50
ATOM	801	CA	LEU	1161	71.522	29.192	47.320	1.00	26.61
ATOM	802	CB	LEU	1161	70.140	29.752	47.670	1.00	26.28
ATOM	803	CG	LEU	1161	69.679	31.031	46.958	1.00	28.68
ATOM	804	CD1	LEU	1161	69.484	30.775	45.469	1.00	29.40
ATOM	805	CD2	LEU	1161	68.392	31.543	47.585	1.00	26.34
ATOM	806	C	LEU	1161	72.054	28.374	48.495	1.00	26.66
ATOM	807	O	LEU	1161	72.247	28.905	49.588	1.00	28.59
ATOM	808	N	ALA	1162	72.297	27.089	48.275	1.00	26.43
ATOM	809	CA	ALA	1162	72.790	26.213	49.330	1.00	26.08
ATOM	810	CB	ALA	1162	72.854	24.773	48.833	1.00	27.54

FIGURE 3 (CONT.)

ATOM	811	C	ALA	1162	74.148	26.638	49.878	1.00	26.55
ATOM	812	O	ALA	1162	75.035	27.049	49.132	1.00	25.22
ATOM	813	N	GLY	1163	74.294	26.505	51.193	1.00	26.94
ATOM	814	CA	GLY	1163	75.526	26.857	51.869	1.00	24.56
ATOM	815	C	GLY	1163	75.724	28.351	52.043	1.00	25.00
ATOM	816	O	GLY	1163	76.767	28.771	52.529	1.00	26.71
ATOM	817	N	SER	1164	74.718	29.151	51.704	1.00	23.80
ATOM	818	CA	SER	1164	74.839	30.597	51.805	1.00	23.26
ATOM	819	CB	SER	1164	74.376	31.267	50.503	1.00	23.11
ATOM	820	OG	SER	1164	75.068	30.759	49.372	1.00	25.78
ATOM	821	C	SER	1164	74.115	31.243	52.968	1.00	23.96
ATOM	822	O	SER	1164	74.153	32.466	53.102	1.00	26.14
ATOM	823	N	SER	1165	73.412	30.474	53.789	1.00	25.28
ATOM	824	CA	SER	1165	72.719	31.113	54.905	1.00	26.92
ATOM	825	CB	SER	1165	71.788	30.142	55.647	1.00	29.04
ATOM	826	OG	SER	1165	72.468	28.977	56.096	1.00	35.95
ATOM	827	C	SER	1165	73.790	31.695	55.820	1.00	24.96
ATOM	828	O	SER	1165	74.785	31.036	56.126	1.00	25.60
ATOM	829	N	GLY	1166	73.610	32.951	56.193	1.00	23.93
ATOM	830	CA	GLY	1166	74.582	33.630	57.026	1.00	22.49
ATOM	831	C	GLY	1166	75.176	34.762	56.207	1.00	22.45
ATOM	832	O	GLY	1166	75.788	35.677	56.752	1.00	20.96
ATOM	833	N	GLY	1167	74.965	34.692	54.892	1.00	22.45
ATOM	834	CA	GLY	1167	75.452	35.697	53.964	1.00	22.73
ATOM	835	C	GLY	1167	74.687	37.003	54.055	1.00	21.55
ATOM	836	O	GLY	1167	73.648	37.067	54.712	1.00	21.50
ATOM	837	N	PRO	1168	75.161	38.061	53.384	1.00	20.49
ATOM	838	CD	PRO	1168	76.450	38.180	52.673	1.00	18.54
ATOM	839	CA	PRO	1168	74.478	39.354	53.439	1.00	20.96
ATOM	840	CB	PRO	1168	75.638	40.333	53.300	1.00	17.41
ATOM	841	CG	PRO	1168	76.463	39.663	52.235	1.00	16.92
ATOM	842	C	PRO	1168	73.424	39.644	52.368	1.00	21.87
ATOM	843	O	PRO	1168	73.480	39.127	51.251	1.00	23.31
ATOM	844	N	LEU	1169	72.472	40.496	52.731	1.00	20.95
ATOM	845	CA	LEU	1169	71.441	40.950	51.818	1.00	20.67
ATOM	846	CB	LEU	1169	70.045	40.673	52.381	1.00	22.16
ATOM	847	CG	LEU	1169	69.367	39.460	51.733	1.00	23.29
ATOM	848	CD1	LEU	1169	68.426	38.826	52.686	1.00	25.16
ATOM	849	CD2	LEU	1169	68.652	39.858	50.459	1.00	24.84
ATOM	850	C	LEU	1169	71.751	42.432	51.781	1.00	20.26
ATOM	851	O	LEU	1169	71.537	43.142	52.761	1.00	20.99
ATOM	852	N	LEU	1170	72.369	42.855	50.686	1.00	20.65
ATOM	853	CA	LEU	1170	72.812	44.230	50.477	1.00	20.86
ATOM	854	CB	LEU	1170	74.097	44.217	49.647	1.00	18.73
ATOM	855	CG	LEU	1170	75.246	43.277	50.028	1.00	19.61
ATOM	856	CD1	LEU	1170	76.349	43.392	48.987	1.00	17.63
ATOM	857	CD2	LEU	1170	75.772	43.597	51.419	1.00	15.34
ATOM	858	C	LEU	1170	71.820	45.149	49.774	1.00	22.02
ATOM	859	O	LEU	1170	71.111	44.729	48.868	1.00	25.14
ATOM	860	N	CYS	1171	71.801	46.414	50.171	1.00	22.01
ATOM	861	CA	CYS	1171	70.930	47.395	49.543	1.00	22.45

FIGURE 3 (CONT.)

ATOM	862	CB	CYS	1171	70.628	48.524	50.531	1.00	22.30
ATOM	863	SG	CYS	1171	71.982	49.681	50.780	1.00	26.39
ATOM	864	C	CYS	1171	71.712	47.929	48.332	1.00	23.53
ATOM	865	O	CYS	1171	72.858	47.527	48.110	1.00	22.06
ATOM	866	N	PRO	1172	71.124	48.850	47.542	1.00	25.28
ATOM	867	CD	PRO	1172	69.721	49.317	47.553	1.00	23.57
ATOM	868	CA	PRO	1172	71.830	49.396	46.371	1.00	23.81
ATOM	869	CB	PRO	1172	70.831	50.418	45.834	1.00	22.44
ATOM	870	CG	PRO	1172	69.517	49.769	46.131	1.00	21.24
ATOM	871	C	PRO	1172	73.188	50.054	46.661	1.00	24.42
ATOM	872	O	PRO	1172	73.981	50.288	45.746	1.00	25.44
ATOM	873	N	ALA	1173	73.446	50.366	47.927	1.00	23.25
ATOM	874	CA	ALA	1173	74.691	51.010	48.333	1.00	22.05
ATOM	875	CB	ALA	1173	74.381	52.102	49.356	1.00	19.70
ATOM	876	C	ALA	1173	75.731	50.033	48.903	1.00	21.83
ATOM	877	O	ALA	1173	76.794	50.449	49.365	1.00	21.56
ATOM	878	N	GLY	1174	75.402	48.745	48.911	1.00	20.69
ATOM	879	CA	GLY	1174	76.313	47.746	49.444	1.00	20.88
ATOM	880	C	GLY	1174	76.286	47.625	50.962	1.00	21.00
ATOM	881	O	GLY	1174	77.148	46.975	51.549	1.00	22.80
ATOM	882	N	HIS	1175	75.310	48.261	51.599	1.00	20.13
ATOM	883	CA	HIS	1175	75.170	48.218	53.052	1.00	19.74
ATOM	884	CB	HIS	1175	74.585	49.533	53.569	1.00	20.08
ATOM	885	CG	HIS	1175	75.465	50.726	53.336	1.00	21.55
ATOM	886	CD2	HIS	1175	76.660	50.845	52.714	1.00	23.16
ATOM	887	ND1	HIS	1175	75.134	51.990	53.775	1.00	22.98
ATOM	888	CE1	HIS	1175	76.088	52.837	53.433	1.00	23.40
ATOM	889	NE2	HIS	1175	77.026	52.168	52.787	1.00	22.42
ATOM	890	C	HIS	1175	74.277	47.049	53.481	1.00	20.52
ATOM	891	O	HIS	1175	73.344	46.679	52.770	1.00	21.87
ATOM	892	N	ALA	1176	74.553	46.492	54.653	1.00	19.06
ATOM	893	CA	ALA	1176	73.809	45.362	55.182	1.00	18.89
ATOM	894	CB	ALA	1176	74.470	44.863	56.442	1.00	18.59
ATOM	895	C	ALA	1176	72.353	45.643	55.475	1.00	21.37
ATOM	896	O	ALA	1176	72.031	46.496	56.304	1.00	21.49
ATOM	897	N	VAL	1177	71.473	44.897	54.817	1.00	22.39
ATOM	898	CA	VAL	1177	70.035	45.024	55.023	1.00	21.72
ATOM	899	CB	VAL	1177	69.246	44.821	53.703	1.00	22.74
ATOM	900	CG1	VAL	1177	67.741	44.788	53.975	1.00	22.68
ATOM	901	CG2	VAL	1177	69.582	45.930	52.720	1.00	20.67
ATOM	902	C	VAL	1177	69.634	43.949	56.027	1.00	21.01
ATOM	903	O	VAL	1177	68.814	44.182	56.915	1.00	22.35
ATOM	904	N	GLY	1178	70.245	42.777	55.891	1.00	20.58
ATOM	905	CA	GLY	1178	69.968	41.668	56.782	1.00	19.29
ATOM	906	C	GLY	1178	70.865	40.491	56.460	1.00	20.72
ATOM	907	O	GLY	1178	71.693	40.564	55.545	1.00	20.77
ATOM	908	N	LEU	1179	70.752	39.436	57.260	1.00	23.38
ATOM	909	CA	LEU	1179	71.521	38.208	57.066	1.00	24.90
ATOM	910	CB	LEU	1179	72.001	37.651	58.408	1.00	27.14
ATOM	911	CG	LEU	1179	73.435	37.842	58.896	1.00	27.77
ATOM	912	CD1	LEU	1179	73.765	39.313	58.996	1.00	29.16

ATOM	913	CD2	LEU	1179	73.573	37.177	60.250	1.00	27.55
ATOM	914	C	LEU	1179	70.578	37.189	56.461	1.00	25.10
ATOM	915	O	LEU	1179	69.475	37.000	56.964	1.00	26.82
ATOM	916	N	PHE	1180	70.987	36.552	55.375	1.00	25.52
ATOM	917	CA	PHE	1180	70.163	35.536	54.744	1.00	26.02
ATOM	918	CB	PHE	1180	70.861	35.030	53.485	1.00	26.33
ATOM	919	CG	PHE	1180	70.193	33.858	52.841	1.00	25.63
ATOM	920	CD1	PHE	1180	68.809	33.754	52.804	1.00	24.18
ATOM	921	CD2	PHE	1180	70.961	32.855	52.258	1.00	26.86
ATOM	922	CE1	PHE	1180	68.203	32.669	52.196	1.00	26.34
ATOM	923	CE2	PHE	1180	70.359	31.760	51.646	1.00	28.46
ATOM	924	CZ	PHE	1180	68.978	31.667	51.614	1.00	27.68
ATOM	925	C	PHE	1180	69.947	34.403	55.751	1.00	27.04
ATOM	926	O	PHE	1180	70.904	33.763	56.200	1.00	28.87
ATOM	927	N	ARG	1181	68.692	34.197	56.135	1.00	27.75
ATOM	928	CA	ARG	1181	68.335	33.168	57.105	1.00	28.04
ATOM	929	CB	ARG	1181	67.193	33.647	58.014	1.00	28.31
ATOM	930	CG	ARG	1181	66.773	32.609	59.047	1.00	30.17
ATOM	931	CD	ARG	1181	65.340	32.795	59.494	1.00	33.18
ATOM	932	NE	ARG	1181	65.225	33.558	60.730	1.00	37.63
ATOM	933	CZ	ARG	1181	64.538	34.694	60.858	1.00	40.99
ATOM	934	NH1	ARG	1181	63.900	35.226	59.818	1.00	40.68
ATOM	935	NH2	ARG	1181	64.455	35.281	62.048	1.00	42.67
ATOM	936	C	ARG	1181	67.962	31.827	56.477	1.00	28.46
ATOM	937	O	ARG	1181	68.499	30.784	56.872	1.00	30.26
ATOM	938	N	ALA	1182	67.046	31.838	55.514	1.00	27.65
ATOM	939	CA	ALA	1182	66.637	30.589	54.887	1.00	26.77
ATOM	940	CB	ALA	1182	65.686	29.841	55.794	1.00	28.57
ATOM	941	C	ALA	1182	66.002	30.777	53.529	1.00	26.90
ATOM	942	O	ALA	1182	65.457	31.842	53.223	1.00	24.79
ATOM	943	N	ALA	1183	66.085	29.727	52.720	1.00	27.64
ATOM	944	CA	ALA	1183	65.519	29.714	51.382	1.00	29.29
ATOM	945	CB	ALA	1183	66.356	28.821	50.469	1.00	28.99
ATOM	946	C	ALA	1183	64.080	29.207	51.433	1.00	31.69
ATOM	947	O	ALA	1183	63.803	28.136	51.992	1.00	31.90
ATOM	948	N	VAL	1184	63.170	30.012	50.893	1.00	32.81
ATOM	949	CA	VAL	1184	61.751	29.681	50.833	1.00	32.42
ATOM	950	CB	VAL	1184	60.893	30.928	51.005	1.00	30.12
ATOM	951	CG1	VAL	1184	59.440	30.583	50.781	1.00	32.26
ATOM	952	CG2	VAL	1184	61.106	31.522	52.380	1.00	30.64
ATOM	953	C	VAL	1184	61.498	29.131	49.441	1.00	33.36
ATOM	954	O	VAL	1184	61.370	29.894	48.478	1.00	32.09
ATOM	955	N	CYS	1185	61.403	27.816	49.326	1.00	35.08
ATOM	956	CA	CYS	1185	61.211	27.215	48.017	1.00	39.13
ATOM	957	CB	CYS	1185	62.486	26.482	47.601	1.00	41.48
ATOM	958	SG	CYS	1185	63.419	25.872	48.998	1.00	44.16
ATOM	959	C	CYS	1185	60.020	26.297	47.822	1.00	38.16
ATOM	960	O	CYS	1185	59.487	25.720	48.772	1.00	36.83
ATOM	961	N	THR	1186	59.574	26.236	46.571	1.00	38.73
ATOM	962	CA	THR	1186	58.469	25.385	46.185	1.00	37.64
ATOM	963	CB	THR	1186	57.582	26.052	45.133	1.00	33.24

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FIGURE 3 (CONT.)

ATOM	964	OG1	THR	1186	57.162	27.327	45.617	1.00	31.32
ATOM	965	CG2	THR	1186	56.340	25.228	44.896	1.00	35.61
ATOM	966	C	THR	1186	59.040	24.049	45.703	1.00	40.01
ATOM	967	O	THR	1186	59.763	23.394	46.453	1.00	43.80
ATOM	968	N	ARG	1187	58.815	23.666	44.454	1.00	40.59
ATOM	969	CA	ARG	1187	59.313	22.371	44.016	1.00	42.08
ATOM	970	CB	ARG	1187	58.452	21.812	42.879	1.00	44.63
ATOM	971	CG	ARG	1187	56.993	21.591	43.280	1.00	45.00
ATOM	972	CD	ARG	1187	56.253	20.703	42.298	1.00	45.42
ATOM	973	NE	ARG	1187	56.736	19.327	42.361	1.00	47.14
ATOM	974	CZ	ARG	1187	57.309	18.683	41.348	1.00	48.66
ATOM	975	NH1	ARG	1187	57.475	19.287	40.175	1.00	49.91
ATOM	976	NH2	ARG	1187	57.731	17.433	41.511	1.00	49.91
ATOM	977	C	ARG	1187	60.788	22.349	43.668	1.00	42.04
ATOM	978	O	ARG	1187	61.165	22.021	42.545	1.00	44.12
ATOM	979	N	GLY	1188	61.623	22.687	44.647	1.00	41.58
ATOM	980	CA	GLY	1188	63.060	22.692	44.435	1.00	40.35
ATOM	981	C	GLY	1188	63.591	24.022	43.935	1.00	39.09
ATOM	982	O	GLY	1188	64.800	24.235	43.881	1.00	40.73
ATOM	983	N	VAL	1189	62.692	24.921	43.561	1.00	36.60
ATOM	984	CA	VAL	1189	63.097	26.220	43.069	1.00	35.55
ATOM	985	CB	VAL	1189	62.290	26.614	41.837	1.00	34.59
ATOM	986	CG1	VAL	1189	62.634	28.026	41.401	1.00	36.44
ATOM	987	CG2	VAL	1189	62.579	25.646	40.716	1.00	35.37
ATOM	988	C	VAL	1189	62.928	27.276	44.145	1.00	36.38
ATOM	989	O	VAL	1189	61.834	27.450	44.677	1.00	37.93
ATOM	990	N	ALA	1190	64.027	27.928	44.510	1.00	35.83
ATOM	991	CA	ALA	1190	64.002	28.983	45.513	1.00	34.95
ATOM	992	CB	ALA	1190	65.400	29.240	46.045	1.00	34.41
ATOM	993	C	ALA	1190	63.465	30.228	44.827	1.00	35.05
ATOM	994	O	ALA	1190	64.062	30.715	43.865	1.00	35.76
ATOM	995	N	LYS	1191	62.321	30.717	45.292	1.00	34.34
ATOM	996	CA	LYS	1191	61.710	31.907	44.709	1.00	33.55
ATOM	997	CB	LYS	1191	60.252	31.636	44.321	1.00	36.37
ATOM	998	CG	LYS	1191	60.037	30.443	43.404	1.00	38.02
ATOM	999	CD	LYS	1191	58.577	30.318	43.028	1.00	41.03
ATOM	1000	CE	LYS	1191	58.333	29.133	42.108	1.00	45.01
ATOM	1001	NZ	LYS	1191	56.902	29.078	41.674	1.00	45.80
ATOM	1002	C	LYS	1191	61.761	33.071	45.692	1.00	33.05
ATOM	1003	O	LYS	1191	61.652	34.231	45.298	1.00	36.29
ATOM	1004	N	ALA	1192	61.896	32.767	46.976	1.00	30.97
ATOM	1005	CA	ALA	1192	61.955	33.809	47.985	1.00	28.85
ATOM	1006	CB	ALA	1192	60.615	33.971	48.684	1.00	28.99
ATOM	1007	C	ALA	1192	63.051	33.494	48.984	1.00	28.42
ATOM	1008	O	ALA	1192	63.596	32.384	49.009	1.00	27.40
ATOM	1009	N	VAL	1193	63.299	34.452	49.863	1.00	27.93
ATOM	1010	CA	VAL	1193	64.355	34.356	50.847	1.00	27.23
ATOM	1011	CB	VAL	1193	65.569	35.180	50.329	1.00	27.43
ATOM	1012	CG1	VAL	1193	66.002	36.251	51.317	1.00	26.78
ATOM	1013	CG2	VAL	1193	66.696	34.258	49.948	1.00	26.32
ATOM	1014	C	VAL	1193	63.858	34.863	52.204	1.00	28.65

FIGURE 3 (CONT.)

ATOM	1015	O	VAL	1193	63.059	35.803	52.281	1.00	29.70
ATOM	1016	N	ASP	1194	64.336	34.233	53.268	1.00	29.83
ATOM	1017	CA	ASP	1194	63.961	34.593	54.634	1.00	31.77
ATOM	1018	CB	ASP	1194	63.611	33.308	55.403	1.00	35.32
ATOM	1019	CG	ASP	1194	62.533	33.513	56.461	1.00	39.12
ATOM	1020	OD1	ASP	1194	62.701	32.961	57.574	1.00	40.47
ATOM	1021	OD2	ASP	1194	61.508	34.176	56.169	1.00	39.60
ATOM	1022	C	ASP	1194	65.218	35.227	55.226	1.00	29.50
ATOM	1023	O	ASP	1194	66.317	34.724	54.995	1.00	30.45
ATOM	1024	N	PHE	1195	65.092	36.322	55.966	1.00	27.58
ATOM	1025	CA	PHE	1195	66.292	36.927	56.537	1.00	25.93
ATOM	1026	CB	PHE	1195	66.981	37.869	55.532	1.00	21.65
ATOM	1027	CG	PHE	1195	66.204	39.118	55.204	1.00	17.29
ATOM	1028	CD1	PHE	1195	66.358	40.267	55.969	1.00	17.07
ATOM	1029	CD2	PHE	1195	65.363	39.162	54.100	1.00	17.69
ATOM	1030	CE1	PHE	1195	65.689	41.447	55.644	1.00	17.82
ATOM	1031	CE2	PHE	1195	64.685	40.343	53.761	1.00	19.76
ATOM	1032	CZ	PHE	1195	64.849	41.491	54.538	1.00	18.59
ATOM	1033	C	PHE	1195	66.140	37.590	57.897	1.00	25.99
ATOM	1034	O	PHE	1195	65.034	37.746	58.404	1.00	27.20
ATOM	1035	N	ILE	1196	67.283	37.916	58.496	1.00	26.69
ATOM	1036	CA	ILE	1196	67.389	38.562	59.804	1.00	25.40
ATOM	1037	CB	ILE	1196	68.535	37.900	60.617	1.00	23.91
ATOM	1038	CG2	ILE	1196	68.599	38.457	62.027	1.00	22.64
ATOM	1039	CG1	ILE	1196	68.357	36.381	60.645	1.00	20.68
ATOM	1040	CD1	ILE	1196	69.570	35.656	61.152	1.00	20.36
ATOM	1041	C	ILE	1196	67.777	40.026	59.548	1.00	28.07
ATOM	1042	O	ILE	1196	68.907	40.309	59.147	1.00	31.19
ATOM	1043	N	PRO	1197	66.853	40.972	59.757	1.00	28.04
ATOM	1044	CD	PRO	1197	65.466	40.830	60.225	1.00	27.62
ATOM	1045	CA	PRO	1197	67.187	42.382	59.521	1.00	29.04
ATOM	1046	CB	PRO	1197	65.851	43.087	59.764	1.00	27.29
ATOM	1047	CG	PRO	1197	65.177	42.204	60.758	1.00	27.91
ATOM	1048	C	PRO	1197	68.296	42.924	60.437	1.00	30.39
ATOM	1049	O	PRO	1197	68.445	42.469	61.571	1.00	30.42
ATOM	1050	N	VAL	1198	69.060	43.904	59.950	1.00	32.28
ATOM	1051	CA	VAL	1198	70.149	44.497	60.738	1.00	32.71
ATOM	1052	CB	VAL	1198	70.968	45.569	59.977	1.00	31.13
ATOM	1053	CG1	VAL	1198	71.893	44.906	58.992	1.00	32.44
ATOM	1054	CG2	VAL	1198	70.060	46.576	59.294	1.00	30.27
ATOM	1055	C	VAL	1198	69.706	45.106	62.046	1.00	33.07
ATOM	1056	O	VAL	1198	70.494	45.192	62.982	1.00	34.24
ATOM	1057	N	GLU	1199	68.459	45.557	62.112	1.00	34.76
ATOM	1058	CA	GLU	1199	67.942	46.133	63.348	1.00	35.58
ATOM	1059	CB	GLU	1199	66.502	46.601	63.167	1.00	38.30
ATOM	1060	CG	GLU	1199	66.347	47.817	62.251	1.00	43.36
ATOM	1061	CD	GLU	1199	66.682	47.546	60.781	1.00	44.71
ATOM	1062	OE1	GLU	1199	67.295	48.437	60.157	1.00	46.89
ATOM	1063	OE2	GLU	1199	66.319	46.470	60.248	1.00	43.96
ATOM	1064	C	GLU	1199	68.035	45.092	64.465	1.00	35.11
ATOM	1065	O	GLU	1199	68.357	45.424	65.599	1.00	35.89

FIGURE 3 (CONT.)

ATOM	1066	N	ASN	1200	67.827	43.823	64.126	1.00	34.53
ATOM	1067	CA	ASN	1200	67.918	42.750	65.108	1.00	34.98
ATOM	1068	CB	ASN	1200	67.515	41.414	64.486	1.00	36.70
ATOM	1069	CG	ASN	1200	66.017	41.289	64.286	1.00	40.49
ATOM	1070	OD1	ASN	1200	65.442	40.231	64.528	1.00	43.89
ATOM	1071	ND2	ASN	1200	65.377	42.358	63.827	1.00	40.79
ATOM	1072	C	ASN	1200	69.345	42.663	65.640	1.00	35.32
ATOM	1073	O	ASN	1200	69.561	42.654	66.852	1.00	35.57
ATOM	1074	N	LEU	1201	70.319	42.635	64.733	1.00	34.45
ATOM	1075	CA	LEU	1201	71.727	42.568	65.124	1.00	32.80
ATOM	1076	CB	LEU	1201	72.643	42.631	63.900	1.00	31.13
ATOM	1077	CG	LEU	1201	72.856	41.383	63.053	1.00	30.40
ATOM	1078	CD1	LEU	1201	71.547	40.751	62.648	1.00	31.05
ATOM	1079	CD2	LEU	1201	73.654	41.764	61.833	1.00	30.17
ATOM	1080	C	LEU	1201	72.026	43.749	66.028	1.00	33.31
ATOM	1081	O	LEU	1201	72.535	43.585	67.135	1.00	33.72
ATOM	1082	N	GLU	1202	71.653	44.933	65.558	1.00	33.90
ATOM	1083	CA	GLU	1202	71.861	46.171	66.294	1.00	35.75
ATOM	1084	CB	GLU	1202	71.292	47.351	65.500	1.00	34.70
ATOM	1085	CG	GLU	1202	72.029	47.574	64.190	1.00	37.02
ATOM	1086	CD	GLU	1202	71.347	48.547	63.247	1.00	40.33
ATOM	1087	OE1	GLU	1202	71.990	48.934	62.256	1.00	43.28
ATOM	1088	OE2	GLU	1202	70.175	48.924	63.462	1.00	44.53
ATOM	1089	C	GLU	1202	71.285	46.122	67.713	1.00	37.01
ATOM	1090	O	GLU	1202	71.977	46.459	68.673	1.00	38.58
ATOM	1091	N	THR	1203	70.043	45.672	67.855	1.00	36.83
ATOM	1092	CA	THR	1203	69.435	45.592	69.174	1.00	38.22
ATOM	1093	CB	THR	1203	67.956	45.209	69.099	1.00	38.67
ATOM	1094	OG1	THR	1203	67.828	43.951	68.434	1.00	42.02
ATOM	1095	CG2	THR	1203	67.168	46.264	68.352	1.00	38.87
ATOM	1096	C	THR	1203	70.156	44.548	70.001	1.00	39.56
ATOM	1097	O	THR	1203	70.425	44.764	71.180	1.00	40.65
ATOM	1098	N	THR	1204	70.479	43.421	69.370	1.00	40.29
ATOM	1099	CA	THR	1204	71.180	42.328	70.040	1.00	40.51
ATOM	1100	CB	THR	1204	71.409	41.146	69.075	1.00	39.96
ATOM	1101	OG1	THR	1204	70.150	40.520	68.785	1.00	37.72
ATOM	1102	CG2	THR	1204	72.353	40.120	69.677	1.00	41.21
ATOM	1103	C	THR	1204	72.492	42.818	70.648	1.00	41.33
ATOM	1104	O	THR	1204	72.932	42.322	71.684	1.00	42.16
ATOM	1105	N	MET	1205	73.101	43.810	70.012	1.00	42.92
ATOM	1106	CA	MET	1205	74.338	44.395	70.510	1.00	44.88
ATOM	1107	CB	MET	1205	75.064	45.136	69.388	1.00	43.43
ATOM	1108	CG	MET	1205	75.778	44.265	68.388	1.00	41.30
ATOM	1109	SD	MET	1205	76.649	45.304	67.195	1.00	38.98
ATOM	1110	CE	MET	1205	75.690	45.025	65.732	1.00	39.73
ATOM	1111	C	MET	1205	74.008	45.401	71.612	1.00	48.30
ATOM	1112	O	MET	1205	74.680	46.434	71.732	1.00	50.45
ATOM	1113	N	ALA	1206	72.985	45.106	72.415	1.00	51.29
ATOM	1114	CA	ALA	1206	72.560	46.001	73.494	1.00	52.72
ATOM	1115	CB	ALA	1206	71.741	47.167	72.919	1.00	51.79
ATOM	1116	C	ALA	1206	71.746	45.253	74.550	1.00	52.50

FIGURE 3 (CONT.)

ATOM 1117   O   ALA   1206   70.842   44.487   74.147   1.00   52.28

sNS4ACOORDINATES   (Complex A)

	Atom Type	Resid	#	X	Y	Z	OCC	B	
ATOM 2427	N	GLY	1678	82.660	20.678	69.142	1.00	47.82	
ATOM 2428	CA	GLY	1678	83.325	21.195	67.901	1.00	47.45	
ATOM 2429	C	GLY	1678	83.444	22.729	67.863	1.00	42.58	
ATOM 2430	O	GLY	1678	83.086	23.435	68.815	1.00	46.32	
ATOM 2431	N	SER	1679	83.951	23.237	66.745	1.00	39.26	
ATOM 2432	CA	SER	1679	84.188	24.669	66.594	1.00	35.38	
ATOM 2433	CB	SER	1679	85.628	24.981	67.011	1.00	34.24	
ATOM 2434	OG	SER	1679	85.746	26.265	67.587	1.00	33.09	
ATOM 2435	C	SER	1679	83.965	25.057	65.134	1.00	32.76	
ATOM 2436	O	SER	1679	84.084	24.218	64.240	1.00	34.29	
ATOM 2437	N	VAL	1680	83.594	26.307	64.894	1.00	29.61	
ATOM 2438	CA	VAL	1680	83.365	26.784	63.533	1.00	27.92	
ATOM 2439	CB	VAL	1680	82.341	27.936	63.495	1.00	27.03	
ATOM 2440	CG1	VAL	1680	81.995	28.277	62.069	1.00	26.39	
ATOM 2441	CG2	VAL	1680	81.099	27.569	64.277	1.00	27.69	
ATOM 2442	C	VAL	1680	84.692	27.311	63.007	1.00	26.65	
ATOM 2443	O	VAL	1680	85.349	28.115	63.666	1.00	28.02	
ATOM 2444	N	VAL	1681	85.108	26.844	61.842	1.00	24.80	
ATOM 2445	CA	VAL	1681	86.364	27.300	61.278	1.00	23.49	
ATOM 2446	CB	VAL	1681	87.331	26.117	61.027	1.00	23.05	
ATOM 2447	CG1	VAL	1681	87.591	25.384	62.314	1.00	21.97	
ATOM 2448	CG2	VAL	1681	86.751	25.153	60.018	1.00	24.91	
ATOM 2449	C	VAL	1681	86.106	28.061	59.985	1.00	22.71	
ATOM 2450	O	VAL	1681	85.156	27.762	59.261	1.00	22.32	
ATOM 2451	N	ILE	1682	86.923	29.077	59.729	1.00	22.79	
ATOM 2452	CA	ILE	1682	86.809	29.899	58.528	1.00	19.66	
ATOM 2453	CB	ILE	1682	87.309	31.332	58.811	1.00	16.80	
ATOM 2454	CG2	ILE	1682	87.324	32.164	57.540	1.00	16.76	
ATOM 2455	CG1	ILE	1682	86.417	31.981	59.875	1.00	13.77	
ATOM 2456	CD1	ILE	1682	86.965	33.244	60.432	1.00	9.56	
ATOM 2457	C	ILE	1682	87.627	29.247	57.418	1.00	19.97	
ATOM 2458	O	ILE	1682	88.844	29.115	57.522	1.00	20.81	
ATOM 2459	N	VAL	1683	86.946	28.826	56.361	1.00	20.17	
ATOM 2460	CA	VAL	1683	87.599	28.157	55.253	1.00	18.67	
ATOM 2461	CB	VAL	1683	86.827	26.867	54.857	1.00	20.13	
ATOM 2462	CG1	VAL	1683	86.595	25.992	56.091	1.00	19.43	
ATOM 2463	CG2	VAL	1683	85.511	27.205	54.188	1.00	21.44	
ATOM 2464	C	VAL	1683	87.785	29.039	54.027	1.00	17.87	
ATOM 2465	O	VAL	1683	88.279	28.592	52.993	1.00	19.88	
ATOM 2466	N	GLY	1684	87.400	30.297	54.135	1.00	16.04	
ATOM 2467	CA	GLY	1684	87.547	31.186	53.005	1.00	13.85	
ATOM 2468	C	GLY	1684	87.006	32.540	53.374	1.00	14.18	
ATOM 2469	O	GLY	1684	86.476	32.709	54.473	1.00	11.33	
ATOM 2470	N	ARG	1685	87.119	33.492	52.452	1.00	16.02	

ATOM	2471	CA	ARG	1685	86.660	34.861	52.660	1.00	16.38
ATOM	2472	CB	ARG	1685	87.800	35.715	53.219	1.00	17.53
ATOM	2473	CG	ARG	1685	88.339	35.249	54.559	1.00	18.90
ATOM	2474	CD	ARG	1685	89.566	36.039	54.945	1.00	20.79
ATOM	2475	NE	ARG	1685	90.609	35.890	53.940	1.00	21.09
ATOM	2476	CZ	ARG	1685	91.532	36.808	53.676	1.00	22.64
ATOM	2477	NH1	ARG	1685	91.552	37.957	54.348	1.00	21.65
ATOM	2478	NH2	ARG	1685	92.426	36.581	52.722	1.00	21.05
ATOM	2479	C	ARG	1685	86.180	35.460	51.343	1.00	15.81
ATOM	2480	O	ARG	1685	86.606	35.034	50.273	1.00	17.35
ATOM	2481	N	ILE	1686	85.313	36.464	51.432	1.00	14.82
ATOM	2482	CA	ILE	1686	84.761	37.142	50.267	1.00	13.14
ATOM	2483	CB	ILE	1686	83.249	36.799	50.100	1.00	14.91
ATOM	2484	CG2	ILE	1686	82.530	37.816	49.216	1.00	9.50
ATOM	2485	CG1	ILE	1686	83.098	35.380	49.543	1.00	16.63
ATOM	2486	CD1	ILE	1686	81.686	34.958	49.338	1.00	16.16
ATOM	2487	C	ILE	1686	84.909	38.637	50.472	1.00	13.59
ATOM	2488	O	ILE	1686	84.614	39.142	51.549	1.00	14.05
ATOM	2489	N	VAL	1687	85.412	39.333	49.458	1.00	15.01
ATOM	2490	CA	VAL	1687	85.575	40.786	49.508	1.00	15.16
ATOM	2491	CB	VAL	1687	86.997	41.223	49.052	1.00	15.36
ATOM	2492	CG1	VAL	1687	87.290	40.797	47.611	1.00	12.78
ATOM	2493	CG2	VAL	1687	87.155	42.702	49.214	1.00	15.07
ATOM	2494	C	VAL	1687	84.500	41.372	48.588	1.00	16.77
ATOM	2495	O	VAL	1687	84.556	41.212	47.372	1.00	18.75
ATOM	2496	N	LEU	1688	83.500	42.017	49.174	1.00	16.57
ATOM	2497	CA	LEU	1688	82.394	42.576	48.411	1.00	16.18
ATOM	2498	CB	LEU	1688	81.400	43.254	49.344	1.00	15.30
ATOM	2499	CG	LEU	1688	80.742	42.326	50.369	1.00	14.41
ATOM	2500	CD1	LEU	1688	79.737	43.122	51.173	1.00	12.70
ATOM	2501	CD2	LEU	1688	80.083	41.142	49.672	1.00	10.09
ATOM	2502	C	LEU	1688	82.737	43.502	47.260	1.00	19.55
ATOM	2503	O	LEU	1688	82.047	43.504	46.243	1.00	23.25
ATOM	2504	N	SER	1689	83.803	44.277	47.401	1.00	23.03
ATOM	2505	CA	SER	1689	84.209	45.213	46.353	1.00	21.96
ATOM	2506	CB	SER	1689	84.999	46.366	46.968	1.00	21.45
ATOM	2507	OG	SER	1689	86.151	45.888	47.643	1.00	24.53
ATOM	2508	C	SER	1689	85.031	44.593	45.238	1.00	22.42
ATOM	2509	O	SER	1689	85.306	45.252	44.239	1.00	25.52
ATOM	2510	N	GLY	1690	85.430	43.337	45.409	1.00	21.46
ATOM	2511	CA	GLY	1690	86.242	42.676	44.406	1.00	21.23
ATOM	2512	C	GLY	1690	87.690	43.130	44.463	1.00	23.65
ATOM	2513	O	GLY	1690	88.451	42.922	43.521	1.00	25.98
ATOM	2514	N	LYS	1691	88.082	43.738	45.577	1.00	23.43
ATOM	2515	CA	LYS	1691	89.445	44.224	45.746	1.00	23.50
ATOM	2516	CB	LYS	1691	89.561	44.980	47.067	1.00	21.39
ATOM	2517	CG	LYS	1691	90.907	45.621	47.286	1.00	21.65
ATOM	2518	CD	LYS	1691	90.888	46.513	48.507	1.00	22.73
ATOM	2519	CE	LYS	1691	92.193	47.269	48.654	1.00	23.13
ATOM	2520	NZ	LYS	1691	92.079	48.318	49.700	1.00	27.11
ATOM	2521	C	LYS	1691	90.503	43.116	45.680	1.00	24.67

FIGURE 3 (CONT.)

ATOM	2522	O	LYS	1691	90.440	42.133	46.424	1.00	26.46
ATOM	2523	N	PRO	1692	91.475	43.249	44.765	1.00	25.07
ATOM	2524	CD	PRO	1692	91.517	44.246	43.682	1.00	24.13
ATOM	2525	CA	PRO	1692	92.549	42.270	44.598	1.00	25.54
ATOM	2526	CB	PRO	1692	92.933	42.456	43.143	1.00	22.92
ATOM	2527	CG	PRO	1692	92.815	43.920	42.986	1.00	23.88
ATOM	2528	C	PRO	1692	93.716	42.601	45.516	1.00	27.60
ATOM	2529	O	PRO	1692	93.810	43.716	46.029	1.00	29.48
ATOM	2530	N	ALA	1693	94.570	41.620	45.770	1.00	31.04
ATOM	2531	CA	ALA	1693	95.736	41.833	46.621	1.00	34.86
ATOM	2532	CB	ALA	1693	96.112	40.543	47.326	1.00	35.21
ATOM	2533	C	ALA	1693	96.915	42.354	45.798	1.00	35.37
ATOM	2534	O	ALA	1693	96.891	42.145	44.559	1.00	35.58

<u>tNS3COORDINATES</u> (ComplexB)

	Atom <u>Type</u>	<u>Resid</u>	<u>#</u>	<u>X</u>	<u>Y</u>	<u>Z</u>	<u>OCC</u>	<u>B</u>	
ATOM	1118	N	PRO	1028	74.820	45.651	43.675	1.00	28.69
ATOM	1119	CD	PRO	1028	75.076	44.493	44.550	1.00	28.33
ATOM	1120	CA	PRO	1028	74.869	46.897	44.441	1.00	28.80
ATOM	1121	CB	PRO	1028	74.807	46.400	45.883	1.00	28.68
ATOM	1122	CG	PRO	1028	75.597	45.138	45.819	1.00	27.37
ATOM	1123	C	PRO	1028	76.163	47.662	44.173	1.00	28.69
ATOM	1124	O	PRO	1028	77.141	47.094	43.666	1.00	30.88
ATOM	1125	N	ILE	1029	76.172	48.950	44.500	1.00	25.65
ATOM	1126	CA	ILE	1029	77.359	49.763	44.288	1.00	22.21
ATOM	1127	CB	ILE	1029	77.029	51.251	44.319	1.00	19.66
ATOM	1128	CG2	ILE	1029	78.254	52.059	43.933	1.00	21.71
ATOM	1129	CG1	ILE	1029	75.883	51.554	43.355	1.00	19.62
ATOM	1130	CD1	ILE	1029	75.398	52.960	43.428	1.00	14.82
ATOM	1131	C	ILE	1029	78.383	49.463	45.371	1.00	23.25
ATOM	1132	O	ILE	1029	78.094	49.586	46.559	1.00	25.52
ATOM	1133	N	THR	1030	79.561	49.023	44.951	1.00	23.20
ATOM	1134	CA	THR	1030	80.651	48.725	45.860	1.00	23.22
ATOM	1135	CB	THR	1030	80.916	47.207	45.958	1.00	23.28
ATOM	1136	OG1	THR	1030	81.077	46.659	44.641	1.00	27.79
ATOM	1137	CG2	THR	1030	79.764	46.508	46.652	1.00	24.32
ATOM	1138	C	THR	1030	81.879	49.406	45.277	1.00	23.10
ATOM	1139	O	THR	1030	81.982	49.562	44.059	1.00	24.23
ATOM	1140	N	ALA	1031	82.821	49.779	46.134	1.00	20.99
ATOM	1141	CA	ALA	1031	84.024	50.456	45.675	1.00	18.06
ATOM	1142	CB	ALA	1031	83.776	51.946	45.635	1.00	19.68
ATOM	1143	C	ALA	1031	85.205	50.172	46.579	1.00	17.02
ATOM	1144	O	ALA	1031	85.036	49.858	47.751	1.00	17.50
ATOM	1145	N	TYR	1032	86.404	50.250	46.028	1.00	16.80
ATOM	1146	CA	TYR	1032	87.597	50.064	46.837	1.00	18.55
ATOM	1147	CB	TYR	1032	88.127	48.633	46.786	1.00	18.83
ATOM	1148	CG	TYR	1032	88.710	48.185	45.466	1.00	15.88
ATOM	1149	CD1	TYR	1032	89.997	48.545	45.088	1.00	13.44

FIGURE 3 (CONT.)

ATOM	1150	CE1	TYR	1032	90.540	48.083	43.899	1.00	15.11
ATOM	1151	CD2	TYR	1032	87.982	47.360	44.619	1.00	15.92
ATOM	1152	CE2	TYR	1032	88.514	46.893	43.436	1.00	15.01
ATOM	1153	CZ	TYR	1032	89.788	47.255	43.075	1.00	15.25
ATOM	1154	OH	TYR	1032	90.298	46.766	41.894	1.00	16.61
ATOM	1155	C	TYR	1032	88.645	51.045	46.368	1.00	18.69
ATOM	1156	O	TYR	1032	88.632	51.462	45.211	1.00	19.25
ATOM	1157	N	ALA	1033	89.525	51.443	47.274	1.00	19.62
ATOM	1158	CA	ALA	1033	90.567	52.394	46.944	1.00	20.61
ATOM	1159	CB	ALA	1033	90.539	53.545	47.922	1.00	18.51
ATOM	1160	C	ALA	1033	91.941	51.738	46.933	1.00	22.70
ATOM	1161	O	ALA	1033	92.142	50.670	47.525	1.00	24.65
ATOM	1162	N	GLN	1034	92.869	52.361	46.215	1.00	23.10
ATOM	1163	CA	GLN	1034	94.236	51.880	46.120	1.00	21.69
ATOM	1164	CB	GLN	1034	94.432	50.971	44.899	1.00	22.35
ATOM	1165	CG	GLN	1034	93.643	49.679	44.895	1.00	23.27
ATOM	1166	CD	GLN	1034	93.927	48.834	43.666	1.00	26.53
ATOM	1167	OE1	GLN	1034	93.982	49.341	42.544	1.00	27.77
ATOM	1168	NE2	GLN	1034	94.119	47.537	43.872	1.00	27.16
ATOM	1169	C	GLN	1034	95.111	53.103	45.955	1.00	22.49
ATOM	1170	O	GLN	1034	94.780	54.005	45.186	1.00	21.85
ATOM	1171	N	GLN	1035	96.194	53.156	46.722	1.00	25.39
ATOM	1172	CA	GLN	1035	97.151	54.253	46.648	1.00	26.92
ATOM	1173	CB	GLN	1035	97.779	54.498	48.013	1.00	29.66
ATOM	1174	CG	GLN	1035	98.985	55.414	47.971	1.00	37.10
ATOM	1175	CD	GLN	1035	98.983	56.413	49.112	1.00	43.12
ATOM	1176	OE1	GLN	1035	98.743	56.056	50.271	1.00	44.84
ATOM	1177	NE2	GLN	1035	99.238	57.678	48.790	1.00	45.69
ATOM	1178	C	GLN	1035	98.234	53.851	45.655	1.00	27.03
ATOM	1179	O	GLN	1035	98.750	52.741	45.726	1.00	29.15
ATOM	1180	N	THR	1036	98.582	54.745	44.738	1.00	26.03
ATOM	1181	CA	THR	1036	99.584	54.437	43.735	1.00	25.05
ATOM	1182	CB	THR	1036	99.094	54.813	42.363	1.00	24.90
ATOM	1183	OG1	THR	1036	98.718	56.192	42.375	1.00	25.74
ATOM	1184	CG2	THR	1036	97.901	53.967	41.988	1.00	23.85
ATOM	1185	C	THR	1036	100.911	55.131	43.976	1.00	26.04
ATOM	1186	O	THR	1036	101.933	54.712	43.427	1.00	27.67
ATOM	1187	N	ARG	1037	100.895	56.232	44.719	1.00	25.73
ATOM	1188	CA	ARG	1037	102.137	56.928	45.023	1.00	25.76
ATOM	1189	CB	ARG	1037	102.596	57.805	43.873	1.00	25.31
ATOM	1190	CG	ARG	1037	101.623	58.844	43.446	1.00	27.06
ATOM	1191	CD	ARG	1037	102.326	59.847	42.575	1.00	27.29
ATOM	1192	NE	ARG	1037	103.303	59.215	41.696	1.00	25.59
ATOM	1193	CZ	ARG	1037	103.077	58.933	40.421	1.00	27.51
ATOM	1194	NH1	ARG	1037	101.893	59.223	39.877	1.00	27.27
ATOM	1195	NH2	ARG	1037	104.048	58.402	39.685	1.00	23.57
ATOM	1196	C	ARG	1037	102.088	57.727	46.303	1.00	26.18
ATOM	1197	O	ARG	1037	101.011	58.021	46.813	1.00	26.32
ATOM	1198	N	GLY	1038	103.266	58.059	46.823	1.00	26.76
ATOM	1199	CA	GLY	1038	103.348	58.806	48.064	1.00	28.78
ATOM	1200	C	GLY	1038	103.715	60.268	47.914	1.00	29.65

FIGURE 3 (CONT.)

ATOM	1201	O	GLY	1038	103.913	60.769	46.805	1.00	30.89
ATOM	1202	N	LEU	1039	103.865	60.929	49.054	1.00	29.52
ATOM	1203	CA	LEU	1039	104.199	62.346	49.135	1.00	30.82
ATOM	1204	CB	LEU	1039	104.550	62.670	50.582	1.00	34.94
ATOM	1205	CG	LEU	1039	104.045	63.977	51.184	1.00	39.14
ATOM	1206	CD1	LEU	1039	103.634	63.744	52.648	1.00	41.57
ATOM	1207	CD2	LEU	1039	105.127	65.038	51.079	1.00	41.24
ATOM	1208	C	LEU	1039	105.342	62.782	48.214	1.00	30.11
ATOM	1209	O	LEU	1039	105.161	63.647	47.354	1.00	29.71
ATOM	1210	N	LEU	1040	106.495	62.136	48.358	1.00	28.91
ATOM	1211	CA	LEU	1040	107.676	62.463	47.568	1.00	27.58
ATOM	1212	CB	LEU	1040	108.878	61.685	48.098	1.00	28.69
ATOM	1213	CG	LEU	1040	110.213	62.413	47.959	1.00	30.89
ATOM	1214	CD1	LEU	1040	110.195	63.632	48.870	1.00	32.42
ATOM	1215	CD2	LEU	1040	111.358	61.492	48.325	1.00	30.06
ATOM	1216	C	LEU	1040	107.524	62.221	46.061	1.00	26.74
ATOM	1217	O	LEU	1040	107.899	63.068	45.242	1.00	28.09
ATOM	1218	N	GLY	1041	106.994	61.062	45.695	1.00	24.50
ATOM	1219	CA	GLY	1041	106.813	60.750	44.291	1.00	23.28
ATOM	1220	C	GLY	1041	105.798	61.679	43.667	1.00	23.92
ATOM	1221	O	GLY	1041	105.922	62.054	42.498	1.00	22.23
ATOM	1222	N	CYS	1042	104.788	62.050	44.449	1.00	23.15
ATOM	1223	CA	CYS	1042	103.751	62.955	43.981	1.00	23.53
ATOM	1224	CB	CYS	1042	102.688	63.138	45.060	1.00	25.84
ATOM	1225	SG	CYS	1042	101.422	64.376	44.680	1.00	27.73
ATOM	1226	C	CYS	1042	104.398	64.289	43.627	1.00	23.74
ATOM	1227	O	CYS	1042	104.253	64.771	42.507	1.00	25.62
ATOM	1228	N	ILE	1043	105.183	64.835	44.555	1.00	23.35
ATOM	1229	CA	ILE	1043	105.878	66.110	44.350	1.00	20.45
ATOM	1230	CB	ILE	1043	106.720	66.484	45.593	1.00	20.32
ATOM	1231	CG2	ILE	1043	107.437	67.810	45.373	1.00	20.94
ATOM	1232	CG1	ILE	1043	105.815	66.571	46.831	1.00	18.68
ATOM	1233	CD1	ILE	1043	106.557	66.802	48.145	1.00	18.48
ATOM	1234	C	ILE	1043	106.765	66.086	43.103	1.00	20.27
ATOM	1235	O	ILE	1043	106.645	66.952	42.242	1.00	23.53
ATOM	1236	N	ILE	1044	107.622	65.077	42.981	1.00	20.30
ATOM	1237	CA	ILE	1044	108.502	64.965	41.817	1.00	19.23
ATOM	1238	CB	ILE	1044	109.370	63.680	41.878	1.00	18.89
ATOM	1239	CG2	ILE	1044	110.205	63.532	40.616	1.00	15.12
ATOM	1240	CG1	ILE	1044	110.276	63.720	43.108	1.00	17.13
ATOM	1241	CD1	ILE	1044	110.979	62.422	43.383	1.00	19.28
ATOM	1242	C	ILE	1044	107.673	64.942	40.541	1.00	20.68
ATOM	1243	O	ILE	1044	107.921	65.721	39.621	1.00	21.41
ATOM	1244	N	THR	1045	106.647	64.094	40.513	1.00	23.02
ATOM	1245	CA	THR	1045	105.779	63.968	39.340	1.00	22.82
ATOM	1246	CB	THR	1045	104.744	62.848	39.515	1.00	22.67
ATOM	1247	OG1	THR	1045	105.415	61.631	39.874	1.00	23.02
ATOM	1248	CG2	THR	1045	103.985	62.630	38.219	1.00	21.21
ATOM	1249	C	THR	1045	105.044	65.260	39.055	1.00	23.69
ATOM	1250	O	THR	1045	104.773	65.583	37.903	1.00	26.48
ATOM	1251	N	SER	1046	104.750	66.013	40.106	1.00	23.58

FIGURE 3 (CONT.)

ATOM	1252	CA	SER	1046	104.043	67.273	39.960	1.00	24.58
ATOM	1253	CB	SER	1046	103.691	67.852	41.331	1.00	25.34
ATOM	1254	OG	SER	1046	102.926	69.034	41.195	1.00	26.40
ATOM	1255	C	SER	1046	104.895	68.264	39.205	1.00	25.37
ATOM	1256	O	SER	1046	104.397	69.000	38.355	1.00	25.66
ATOM	1257	N	LEU	1047	106.183	68.281	39.521	1.00	25.73
ATOM	1258	CA	LEU	1047	107.094	69.204	38.873	1.00	26.65
ATOM	1259	CB	LEU	1047	108.316	69.450	39.759	1.00	26.72
ATOM	1260	CG	LEU	1047	107.985	69.811	41.217	1.00	26.90
ATOM	1261	CD1	LEU	1047	109.237	70.265	41.944	1.00	25.51
ATOM	1262	CD2	LEU	1047	106.920	70.890	41.284	1.00	26.82
ATOM	1263	C	LEU	1047	107.494	68.762	37.466	1.00	27.72
ATOM	1264	O	LEU	1047	107.461	69.561	36.535	1.00	29.56
ATOM	1265	N	THR	1048	107.806	67.483	37.288	1.00	28.48
ATOM	1266	CA	THR	1048	108.203	66.992	35.968	1.00	27.84
ATOM	1267	CB	THR	1048	108.815	65.591	36.046	1.00	26.24
ATOM	1268	OG1	THR	1048	107.818	64.666	36.495	1.00	28.13
ATOM	1269	CG2	THR	1048	110.002	65.580	37.001	1.00	23.61
ATOM	1270	C	THR	1048	107.022	66.936	35.008	1.00	28.29
ATOM	1271	O	THR	1048	107.167	67.168	33.802	1.00	28.96
ATOM	1272	N	GLY	1049	105.860	66.592	35.553	1.00	29.55
ATOM	1273	CA	GLY	1049	104.652	66.490	34.759	1.00	28.26
ATOM	1274	C	GLY	1049	104.582	65.197	33.975	1.00	28.82
ATOM	1275	O	GLY	1049	103.734	65.051	33.096	1.00	27.69
ATOM	1276	N	ARG	1050	105.447	64.242	34.304	1.00	29.15
ATOM	1277	CA	ARG	1050	105.464	62.968	33.595	1.00	30.31
ATOM	1278	CB	ARG	1050	106.852	62.709	33.002	1.00	32.91
ATOM	1279	CG	ARG	1050	106.864	61.866	31.728	1.00	39.62
ATOM	1280	CD	ARG	1050	108.295	61.494	31.320	1.00	46.14
ATOM	1281	NE	ARG	1050	108.577	60.054	31.442	1.00	52.84
ATOM	1282	CZ	ARG	1050	109.518	59.516	32.227	1.00	55.48
ATOM	1283	NH1	ARG	1050	110.290	60.283	32.990	1.00	58.74
ATOM	1284	NH2	ARG	1050	109.730	58.204	32.208	1.00	55.47
ATOM	1285	C	ARG	1050	105.085	61.875	34.586	1.00	29.07
ATOM	1286	O	ARG	1050	105.691	61.751	35.643	1.00	29.25
ATOM	1287	N	ASP	1051	104.040	61.123	34.267	1.00	28.54
ATOM	1288	CA	ASP	1051	103.572	60.054	35.133	1.00	27.21
ATOM	1289	CB	ASP	1051	102.214	60.412	35.729	1.00	28.72
ATOM	1290	CG	ASP	1051	101.694	59.357	36.684	1.00	27.51
ATOM	1291	OD1	ASP	1051	102.495	58.544	37.189	1.00	29.23
ATOM	1292	OD2	ASP	1051	100.478	59.354	36.941	1.00	27.37
ATOM	1293	C	ASP	1051	103.446	58.790	34.320	1.00	28.42
ATOM	1294	O	ASP	1051	102.531	58.658	33.513	1.00	29.82
ATOM	1295	N	LYS	1052	104.359	57.857	34.551	1.00	29.39
ATOM	1296	CA	LYS	1052	104.369	56.596	33.830	1.00	30.29
ATOM	1297	CB	LYS	1052	105.808	56.117	33.647	1.00	32.22
ATOM	1298	CG	LYS	1052	106.598	56.878	32.577	1.00	35.28
ATOM	1299	CD	LYS	1052	106.059	56.579	31.175	1.00	38.64
ATOM	1300	CE	LYS	1052	106.089	55.073	30.869	1.00	41.17
ATOM	1301	NZ	LYS	1052	105.403	54.714	29.588	1.00	42.32
ATOM	1302	C	LYS	1052	103.512	55.485	34.447	1.00	31.22

ATOM	1303	O	LYS	1052	103.356	54.424	33.841	1.00	33.64
ATOM	1304	N	ASN	1053	102.965	55.718	35.641	1.00	29.10
ATOM	1305	CA	ASN	1053	102.123	54.718	36.301	1.00	26.26
ATOM	1306	CB	ASN	1053	101.581	55.233	37.631	1.00	25.64
ATOM	1307	CG	ASN	1053	102.609	55.207	38.727	1.00	23.95
ATOM	1308	OD1	ASN	1053	103.801	55.064	38.468	1.00	26.76
ATOM	1309	ND2	ASN	1053	102.161	55.363	39.963	1.00	22.69
ATOM	1310	C	ASN	1053	100.942	54.380	35.427	1.00	26.87
ATOM	1311	O	ASN	1053	100.483	55.222	34.649	1.00	26.93
ATOM	1312	N	ALA	1054	100.457	53.147	35.545	1.00	27.34
ATOM	1313	CA	ALA	1054	99.301	52.713	34.766	1.00	27.38
ATOM	1314	CB	ALA	1054	99.275	51.196	34.623	1.00	29.92
ATOM	1315	C	ALA	1054	98.056	53.200	35.487	1.00	26.71
ATOM	1316	O	ALA	1054	98.049	53.329	36.720	1.00	26.64
ATOM	1317	N	VAL	1055	97.009	53.474	34.716	1.00	25.91
ATOM	1318	CA	VAL	1055	95.761	53.978	35.269	1.00	24.92
ATOM	1319	CB	VAL	1055	95.262	55.216	34.476	1.00	22.35
ATOM	1320	CG1	VAL	1055	93.954	55.731	35.052	1.00	22.08
ATOM	1321	CG2	VAL	1055	96.296	56.310	34.517	1.00	20.14
ATOM	1322	C	VAL	1055	94.681	52.908	35.257	1.00	24.94
ATOM	1323	O	VAL	1055	94.641	52.064	34.367	1.00	24.51
ATOM	1324	N	GLU	1056	93.826	52.938	36.269	1.00	25.14
ATOM	1325	CA	GLU	1056	92.720	52.008	36.377	1.00	25.82
ATOM	1326	CB	GLU	1056	93.123	50.767	37.163	1.00	28.83
ATOM	1327	CG	GLU	1056	93.973	49.772	36.406	1.00	36.03
ATOM	1328	CD	GLU	1056	93.831	48.360	36.961	1.00	42.08
ATOM	1329	OE1	GLU	1056	93.640	48.210	38.191	1.00	43.57
ATOM	1330	OE2	GLU	1056	93.889	47.398	36.159	1.00	46.03
ATOM	1331	C	GLU	1056	91.614	52.702	37.131	1.00	24.57
ATOM	1332	O	GLU	1056	91.856	53.700	37.810	1.00	26.39
ATOM	1333	N	GLY	1057	90.399	52.189	37.006	1.00	22.01
ATOM	1334	CA	GLY	1057	89.293	52.773	37.737	1.00	20.85
ATOM	1335	C	GLY	1057	88.552	53.902	37.067	1.00	19.15
ATOM	1336	O	GLY	1057	89.013	54.476	36.079	1.00	19.49
ATOM	1337	N	GLU	1058	87.385	54.203	37.631	1.00	19.23
ATOM	1338	CA	GLU	1058	86.479	55.239	37.141	1.00	16.31
ATOM	1339	CB	GLU	1058	85.026	54.871	37.479	1.00	15.32
ATOM	1340	CG	GLU	1058	84.457	53.613	36.792	1.00	15.36
ATOM	1341	CD	GLU	1058	85.101	52.303	37.238	1.00	18.10
ATOM	1342	OE1	GLU	1058	85.591	52.192	38.377	1.00	20.29
ATOM	1343	OE2	GLU	1058	85.118	51.359	36.434	1.00	24.06
ATOM	1344	C	GLU	1058	86.804	56.561	37.803	1.00	15.32
ATOM	1345	O	GLU	1058	86.610	57.623	37.224	1.00	15.89
ATOM	1346	N	VAL	1059	87.292	56.485	39.034	1.00	14.97
ATOM	1347	CA	VAL	1059	87.629	57.661	39.818	1.00	12.63
ATOM	1348	CB	VAL	1059	86.813	57.684	41.136	1.00	9.72
ATOM	1349	CG1	VAL	1059	86.972	59.015	41.839	1.00	10.00
ATOM	1350	CG2	VAL	1059	85.345	57.395	40.862	1.00	7.03
ATOM	1351	C	VAL	1059	89.121	57.661	40.156	1.00	14.78
ATOM	1352	O	VAL	1059	89.656	56.673	40.648	1.00	15.26
ATOM	1353	N	GLN	1060	89.796	58.759	39.845	1.00	16.52

FIGURE 3 (CONT.)

ATOM	1354	CA	GLN	1060	91.212	58.894	40.140	1.00	16.47
ATOM	1355	CB	GLN	1060	91.936	59.556	38.967	1.00	15.66
ATOM	1356	CG	GLN	1060	91.816	58.816	37.670	1.00	17.53
ATOM	1357	CD	GLN	1060	92.215	57.361	37.809	1.00	20.63
ATOM	1358	OE1	GLN	1060	93.215	57.037	38.448	1.00	22.69
ATOM	1359	NE2	GLN	1060	91.424	56.474	37.229	1.00	22.24
ATOM	1360	C	GLN	1060	91.367	59.775	41.372	1.00	18.64
ATOM	1361	O	GLN	1060	90.702	60.801	41.496	1.00	21.76
ATOM	1362	N	ILE	1061	92.175	59.345	42.326	1.00	19.32
ATOM	1363	CA	ILE	1061	92.410	60.171	43.499	1.00	19.78
ATOM	1364	CB	ILE	1061	92.838	59.329	44.718	1.00	18.89
ATOM	1365	CG2	ILE	1061	93.064	60.225	45.926	1.00	18.02
ATOM	1366	CG1	ILE	1061	91.759	58.289	45.033	1.00	16.75
ATOM	1367	CD1	ILE	1061	92.138	57.352	46.120	1.00	14.36
ATOM	1368	C	ILE	1061	93.552	61.068	43.030	1.00	21.51
ATOM	1369	O	ILE	1061	94.615	60.579	42.626	1.00	22.71
ATOM	1370	N	VAL	1062	93.305	62.370	42.979	1.00	21.91
ATOM	1371	CA	VAL	1062	94.321	63.294	42.515	1.00	19.92
ATOM	1372	CB	VAL	1062	93.858	64.075	41.278	1.00	18.17
ATOM	1373	CG1	VAL	1062	93.500	63.117	40.166	1.00	15.34
ATOM	1374	CG2	VAL	1062	92.692	64.977	41.622	1.00	15.73
ATOM	1375	C	VAL	1062	94.776	64.252	43.588	1.00	21.02
ATOM	1376	O	VAL	1062	94.099	64.449	44.593	1.00	22.09
ATOM	1377	N	SER	1063	95.937	64.850	43.367	1.00	22.93
ATOM	1378	CA	SER	1063	96.500	65.776	44.324	1.00	23.94
ATOM	1379	CB	SER	1063	97.290	64.996	45.370	1.00	25.73
ATOM	1380	OG	SER	1063	97.794	65.862	46.369	1.00	32.24
ATOM	1381	C	SER	1063	97.413	66.795	43.673	1.00	23.42
ATOM	1382	O	SER	1063	97.944	66.587	42.578	1.00	20.31
ATOM	1383	N	THR	1064	97.587	67.897	44.382	1.00	26.57
ATOM	1384	CA	THR	1064	98.446	69.005	43.978	1.00	29.88
ATOM	1385	CB	THR	1064	97.629	70.305	43.763	1.00	27.45
ATOM	1386	OG1	THR	1064	97.036	70.707	45.004	1.00	25.21
ATOM	1387	CG2	THR	1064	96.523	70.086	42.751	1.00	26.09
ATOM	1388	C	THR	1064	99.358	69.202	45.194	1.00	32.85
ATOM	1389	O	THR	1064	99.408	68.350	46.086	1.00	34.87
ATOM	1390	N	ALA	1065	100.055	70.326	45.252	1.00	35.39
ATOM	1391	CA	ALA	1065	100.924	70.604	46.388	1.00	35.88
ATOM	1392	CB	ALA	1065	101.866	71.747	46.051	1.00	37.88
ATOM	1393	C	ALA	1065	100.052	70.978	47.578	1.00	35.60
ATOM	1394	O	ALA	1065	100.275	70.537	48.698	1.00	35.43
ATOM	1395	N	THR	1066	99.028	71.772	47.307	1.00	36.74
ATOM	1396	CA	THR	1066	98.119	72.240	48.339	1.00	37.72
ATOM	1397	CB	THR	1066	97.434	73.583	47.895	1.00	39.54
ATOM	1398	OG1	THR	1066	96.431	73.973	48.844	1.00	41.76
ATOM	1399	CG2	THR	1066	96.792	73.444	46.514	1.00	40.92
ATOM	1400	C	THR	1066	97.043	71.261	48.808	1.00	36.34
ATOM	1401	O	THR	1066	96.641	71.307	49.975	1.00	36.42
ATOM	1402	N	GLN	1067	96.608	70.340	47.952	1.00	34.64
ATOM	1403	CA	GLN	1067	95.517	69.461	48.367	1.00	34.70
ATOM	1404	CB	GLN	1067	91.235	70.290	48.381	1.00	36.42

FIGURE 3 (CONT.)

ATOM	1405	CG	GLN	1067	93.980	70.953	47.033	1.00	40.18
ATOM	1406	CD	GLN	1067	92.844	71.952	47.052	1.00	42.84
ATOM	1407	OE1	GLN	1067	91.783	71.704	47.632	1.00	44.48
ATOM	1408	NE2	GLN	1067	93.048	73.080	46.383	1.00	45.42
ATOM	1409	C	GLN	1067	95.263	68.210	47.536	1.00	32.18
ATOM	1410	O	GLN	1067	95.813	68.051	46.449	1.00	32.90
ATOM	1411	N	THR	1068	94.379	67.357	48.054	1.00	29.91
ATOM	1412	CA	THR	1068	93.972	66.108	47.413	1.00	27.99
ATOM	1413	CB	THR	1068	94.296	64.860	48.291	1.00	28.36
ATOM	1414	OG1	THR	1068	95.710	64.751	48.488	1.00	30.82
ATOM	1415	CG2	THR	1068	93.788	63.581	47.636	1.00	26.64
ATOM	1416	C	THR	1068	92.460	66.158	47.248	1.00	25.47
ATOM	1417	O	THR	1068	91.745	66.644	48.126	1.00	25.64
ATOM	1418	N	PHE	1069	91.988	65.670	46.112	1.00	23.13
ATOM	1419	CA	PHE	1069	90.565	65.621	45.801	1.00	20.30
ATOM	1420	CB	PHE	1069	90.060	66.960	45.222	1.00	19.44
ATOM	1421	CG	PHE	1069	91.012	67.618	44.258	1.00	18.91
ATOM	1422	CD1	PHE	1069	90.765	67.593	42.890	1.00	16.69
ATOM	1423	CD2	PHE	1069	92.174	68.237	44.720	1.00	16.99
ATOM	1424	CE1	PHE	1069	91.663	68.165	41.998	1.00	17.12
ATOM	1425	CE2	PHE	1069	93.075	68.811	43.838	1.00	15.95
ATOM	1426	CZ	PHE	1069	92.822	68.775	42.475	1.00	17.86
ATOM	1427	C	PHE	1069	90.340	64.454	44.840	1.00	19.50
ATOM	1428	O	PHE	1069	91.216	63.590	44.687	1.00	18.25
ATOM	1429	N	LEU	1070	89.171	64.402	44.216	1.00	17.14
ATOM	1430	CA	LEU	1070	88.872	63.320	43.297	1.00	16.12
ATOM	1431	CB	LEU	1070	87.699	62.499	43.806	1.00	15.63
ATOM	1432	CG	LEU	1070	87.908	61.837	45.157	1.00	13.76
ATOM	1433	CD1	LEU	1070	86.650	61.104	45.531	1.00	16.70
ATOM	1434	CD2	LEU	1070	89.072	60.890	45.082	1.00	15.02
ATOM	1435	C	LEU	1070	88.545	63.848	41.926	1.00	16.35
ATOM	1436	O	LEU	1070	88.181	65.011	41.774	1.00	18.69
ATOM	1437	N	ALA	1071	88.703	62.989	40.929	1.00	15.91
ATOM	1438	CA	ALA	1071	88.417	63.323	39.544	1.00	15.63
ATOM	1439	CB	ALA	1071	89.701	63.547	38.773	1.00	14.74
ATOM	1440	C	ALA	1071	87.717	62.086	39.050	1.00	16.11
ATOM	1441	O	ALA	1071	88.194	60.981	39.278	1.00	16.97
ATOM	1442	N	THR	1072	86.572	62.273	38.410	1.00	17.64
ATOM	1443	CA	THR	1072	85.764	61.171	37.914	1.00	15.73
ATOM	1444	CB	THR	1072	84.329	61.312	38.416	1.00	15.97
ATOM	1445	OG1	THR	1072	84.344	61.551	39.827	1.00	18.30
ATOM	1446	CG2	THR	1072	83.539	60.052	38.134	1.00	18.15
ATOM	1447	C	THR	1072	85.725	61.166	36.405	1.00	14.68
ATOM	1448	O	THR	1072	85.511	62.197	35.786	1.00	16.38
ATOM	1449	N	CYS	1073	85.890	59.998	35.808	1.00	14.37
ATOM	1450	CA	CYS	1073	85.856	59.895	34.364	1.00	15.72
ATOM	1451	CB	CYS	1073	86.814	58.807	33.889	1.00	17.69
ATOM	1452	SG	CYS	1073	88.536	59.069	34.384	1.00	23.22
ATOM	1453	C	CYS	1073	84.450	59.591	33.878	1.00	16.21
ATOM	1454	O	CYS	1073	83.850	58.601	34.286	1.00	15.04
ATOM	1455	N	ILE	1074	83.907	60.472	33.044	1.00	17.51

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FIGURE 3 (CONT.)

ATOM	1456	CA	ILE	1074	82.578	60.294	32.475	1.00	20.31
ATOM	1457	CB	ILE	1074	81.560	61.315	33.050	1.00	20.77
ATOM	1458	CG2	ILE	1074	80.171	61.053	32.472	1.00	20.99
ATOM	1459	CG1	ILE	1074	81.509	61.221	34.580	1.00	19.74
ATOM	1460	CD1	ILE	1074	80.686	62.297	35.259	1.00	16.17
ATOM	1461	C	ILE	1074	82.716	60.504	30.963	1.00	24.53
ATOM	1462	O	ILE	1074	83.299	61.493	30.521	1.00	28.24
ATOM	1463	N	ASN	1075	82.236	59.543	30.176	1.00	27.13
ATOM	1464	CA	ASN	1075	82.297	59.601	28.708	1.00	25.19
ATOM	1465	CB	ASN	1075	81.193	60.502	28.146	1.00	24.15
ATOM	1466	CG	ASN	1075	79.836	59.845	28.180	1.00	20.59
ATOM	1467	OD1	ASN	1075	79.635	58.844	28.858	1.00	22.02
ATOM	1468	ND2	ASN	1075	78.894	60.406	27.453	1.00	23.38
ATOM	1469	C	ASN	1075	83.642	59.983	28.092	1.00	26.07
ATOM	1470	O	ASN	1075	83.707	60.798	27.164	1.00	29.28
ATOM	1471	N	GLY	1076	84.718	59.394	28.602	1.00	26.05
ATOM	1472	CA	GLY	1076	86.040	59.670	28.059	1.00	23.82
ATOM	1473	C	GLY	1076	86.737	60.935	28.512	1.00	22.44
ATOM	1474	O	GLY	1076	87.779	61.292	27.959	1.00	23.12
ATOM	1475	N	VAL	1077	86.202	61.595	29.534	1.00	22.15
ATOM	1476	CA	VAL	1077	86.799	62.820	30.048	1.00	21.41
ATOM	1477	CB	VAL	1077	85.933	64.056	29.706	1.00	22.29
ATOM	1478	CG1	VAL	1077	86.555	65.329	30.281	1.00	22.38
ATOM	1479	CG2	VAL	1077	85.767	64.180	28.200	1.00	22.13
ATOM	1480	C	VAL	1077	86.950	62.729	31.558	1.00	20.92
ATOM	1481	O	VAL	1077	86.036	62.291	32.256	1.00	22.56
ATOM	1482	N	CYS	1078	88.120	63.112	32.053	1.00	19.00
ATOM	1483	CA	CYS	1078	88.399	63.090	33.482	1.00	18.18
ATOM	1484	CB	CYS	1078	89.886	62.832	33.736	1.00	17.52
ATOM	1485	SG	CYS	1078	90.338	62.568	35.461	1.00	16.09
ATOM	1486	C	CYS	1078	88.008	64.441	34.045	1.00	17.95
ATOM	1487	O	CYS	1078	88.768	65.402	33.962	1.00	21.44
ATOM	1488	N	TRP	1079	86.802	64.513	34.589	1.00	18.33
ATOM	1489	CA	TRP	1079	86.267	65.737	35.164	1.00	14.96
ATOM	1490	CB	TRP	1079	84.744	65.736	35.066	1.00	15.12
ATOM	1491	CG	TRP	1079	84.213	65.817	33.677	1.00	17.41
ATOM	1492	CD2	TRP	1079	84.023	67.007	32.903	1.00	18.04
ATOM	1493	CE2	TRP	1079	83.465	66.619	31.668	1.00	19.10
ATOM	1494	CE3	TRP	1079	84.268	68.369	33.137	1.00	17.65
ATOM	1495	CD1	TRP	1079	83.780	64.781	32.904	1.00	16.78
ATOM	1496	NE1	TRP	1079	83.325	65.254	31.693	1.00	19.80
ATOM	1497	CZ2	TRP	1079	83.146	67.545	30.664	1.00	19.19
ATOM	1498	CZ3	TRP	1079	83.949	69.291	32.139	1.00	15.70
ATOM	1499	CH2	TRP	1079	83.395	68.873	30.921	1.00	16.14
ATOM	1500	C	TRP	1079	86.631	65.895	36.619	1.00	15.06
ATOM	1501	O	TRP	1079	86.701	64.926	37.363	1.00	14.95
ATOM	1502	N	THR	1080	86.851	67.129	37.034	1.00	17.34
ATOM	1503	CA	THR	1080	87.148	67.390	38.421	1.00	19.67
ATOM	1504	CB	THR	1080	88.636	67.201	38.762	1.00	19.66
ATOM	1505	OG1	THR	1080	88.794	67.207	40.187	1.00	18.69
ATOM	1506	CG2	THR	1080	89.475	68.299	38.162	1.00	21.67

FIGURE 3 (CONT.)

ATOM	1507	C	THR	1080	86.663	68.781	38.780	1.00	21.24
ATOM	1508	O	THR	1080	86.113	69.499	37.938	1.00	20.94
ATOM	1509	N	VAL	1081	86.867	69.141	40.039	1.00	23.41
ATOM	1510	CA	VAL	1081	86.444	70.417	40.588	1.00	23.97
ATOM	1511	CB	VAL	1081	86.053	70.200	42.076	1.00	22.41
ATOM	1512	CG1	VAL	1081	87.258	70.300	42.987	1.00	21.40
ATOM	1513	CG2	VAL	1081	84.918	71.094	42.474	1.00	23.79
ATOM	1514	C	VAL	1081	87.519	71.520	40.384	1.00	25.41
ATOM	1515	O	VAL	1081	88.715	71.316	40.632	1.00	24.93
ATOM	1516	N	TYR	1082	87.093	72.683	39.903	1.00	25.72
ATOM	1517	CA	TYR	1082	88.016	73.785	39.643	1.00	25.46
ATOM	1518	CB	TYR	1082	87.321	74.892	38.840	1.00	26.17
ATOM	1519	CG	TYR	1082	88.245	76.005	38.392	1.00	26.30
ATOM	1520	CD1	TYR	1082	88.538	77.075	39.240	1.00	26.95
ATOM	1521	CE1	TYR	1082	89.411	78.092	38.852	1.00	28.63
ATOM	1522	CD2	TYR	1082	88.846	75.973	37.138	1.00	26.52
ATOM	1523	CE2	TYR	1082	89.724	76.982	36.735	1.00	29.11
ATOM	1524	CZ	TYR	1082	90.006	78.038	37.600	1.00	30.48
ATOM	1525	OH	TYR	1082	90.886	79.038	37.222	1.00	31.27
ATOM	1526	C	TYR	1082	88.665	74.349	40.910	1.00	25.31
ATOM	1527	O	TYR	1082	89.793	74.845	40.863	1.00	22.94
ATOM	1528	N	HIS	1083	87.986	74.239	42.049	1.00	24.48
ATOM	1529	CA	HIS	1083	88.568	74.748	43.283	1.00	25.01
ATOM	1530	CB	HIS	1083	87.514	74.963	44.378	1.00	23.89
ATOM	1531	CG	HIS	1083	86.984	73.707	44.999	1.00	27.06
ATOM	1532	CD2	HIS	1083	87.505	72.888	45.948	1.00	28.89
ATOM	1533	ND1	HIS	1083	85.723	73.216	44.727	1.00	29.27
ATOM	1534	CE1	HIS	1083	85.488	72.155	45.479	1.00	28.81
ATOM	1535	NE2	HIS	1083	86.554	71.936	46.229	1.00	30.38
ATOM	1536	C	HIS	1083	89.701	73.853	43.766	1.00	26.93
ATOM	1537	O	HIS	1083	90.266	74.073	44.837	1.00	29.65
ATOM	1538	N	GLY	1084	90.008	72.823	42.985	1.00	25.81
ATOM	1539	CA	GLY	1084	91.082	71.922	43.336	1.00	23.74
ATOM	1540	C	GLY	1084	92.153	71.987	42.266	1.00	21.87
ATOM	1541	O	GLY	1084	93.286	72.360	42.540	1.00	22.00
ATOM	1542	N	ALA	1085	91.771	71.667	41.035	1.00	21.01
ATOM	1543	CA	ALA	1085	92.696	71.662	39.911	1.00	20.52
ATOM	1544	CB	ALA	1085	92.103	70.883	38.752	1.00	18.56
ATOM	1545	C	ALA	1085	93.143	73.034	39.436	1.00	21.49
ATOM	1546	O	ALA	1085	94.273	73.192	39.000	1.00	23.82
ATOM	1547	N	GLY	1086	92.265	74.025	39.498	1.00	22.93
ATOM	1548	CA	GLY	1086	92.641	75.344	39.033	1.00	22.64
ATOM	1549	C	GLY	1086	92.791	75.264	37.526	1.00	25.01
ATOM	1550	O	GLY	1086	91.981	74.631	36.851	1.00	25.80
ATOM	1551	N	THR	1087	93.830	75.876	36.984	1.00	26.41
ATOM	1552	CA	THR	1087	94.032	75.829	35.544	1.00	29.05
ATOM	1553	CB	THR	1087	94.450	77.204	35.003	1.00	32.46
ATOM	1554	OG1	THR	1087	95.572	77.683	35.758	1.00	34.46
ATOM	1555	CG2	THR	1087	93.292	78.209	35.086	1.00	33.93
ATOM	1556	C	THR	1087	95.127	74.846	35.159	1.00	28.61
ATOM	1557	O	THR	1087	95.422	74.679	33.971	1.00	30.95

ATOM	1558	N	ARG	1088	95.689	74.145	36.138	1.00	27.72
ATOM	1559	CA	ARG	1088	96.793	73.247	35.837	1.00	26.27
ATOM	1560	CB	ARG	1088	97.606	72.923	37.083	1.00	25.05
ATOM	1561	CG	ARG	1088	96.830	72.482	38.249	1.00	22.82
ATOM	1562	CD	ARG	1088	97.651	72.707	39.472	1.00	22.84
ATOM	1563	NE	ARG	1088	96.964	73.601	40.382	1.00	26.47
ATOM	1564	CZ	ARG	1088	97.386	73.875	41.607	1.00	28.75
ATOM	1565	NH1	ARG	1088	98.505	73.324	42.068	1.00	31.62
ATOM	1566	NH2	ARG	1088	96.677	74.691	42.375	1.00	29.37
ATOM	1567	C	ARG	1088	96.577	72.014	34.993	1.00	25.66
ATOM	1568	O	ARG	1088	95.448	71.583	34.752	1.00	28.07
ATOM	1569	N	THR	1089	97.694	71.509	34.487	1.00	23.84
ATOM	1570	CA	THR	1089	97.736	70.343	33.633	1.00	23.41
ATOM	1571	CB	THR	1089	99.014	70.390	32.769	1.00	23.85
ATOM	1572	OG1	THR	1089	100.146	70.668	33.602	1.00	24.27
ATOM	1573	CG2	THR	1089	98.916	71.474	31.715	1.00	21.97
ATOM	1574	C	THR	1089	97.742	69.085	34.493	1.00	23.76
ATOM	1575	O	THR	1089	97.876	69.172	35.717	1.00	24.27
ATOM	1576	N	ILE	1090	97.546	67.925	33.869	1.00	21.48
ATOM	1577	CA	ILE	1090	97.570	66.659	34.600	1.00	20.72
ATOM	1578	CB	ILE	1090	96.251	65.811	34.409	1.00	19.48
ATOM	1579	CG2	ILE	1090	96.115	65.296	32.977	1.00	20.97
ATOM	1580	CG1	ILE	1090	96.216	64.642	35.405	1.00	19.86
ATOM	1581	CD1	ILE	1090	94.857	63.936	35.519	1.00	15.19
ATOM	1582	C	ILE	1090	98.803	65.896	34.135	1.00	19.55
ATOM	1583	O	ILE	1090	99.091	65.841	32.940	1.00	17.18
ATOM	1584	N	ALA	1091	99.582	65.395	35.085	1.00	19.06
ATOM	1585	CA	ALA	1091	100.786	64.648	34.750	1.00	17.95
ATOM	1586	CB	ALA	1091	101.558	64.318	36.007	1.00	15.33
ATOM	1587	C	ALA	1091	100.378	63.374	34.036	1.00	19.98
ATOM	1588	O	ALA	1091	99.509	62.643	34.515	1.00	22.10
ATOM	1589	N	SER	1092	100.978	63.116	32.882	1.00	21.44
ATOM	1590	CA	SER	1092	100.667	61.913	32.128	1.00	24.34
ATOM	1591	CB	SER	1092	99.759	62.244	30.941	1.00	24.98
ATOM	1592	OG	SER	1092	100.517	62.642	29.817	1.00	26.24
ATOM	1593	C	SER	1092	101.953	61.271	31.629	1.00	25.86
ATOM	1594	O	SER	1092	103.030	61.838	31.771	1.00	27.85
ATOM	1595	N	PRO	1093	101.862	60.064	31.060	1.00	27.32
ATOM	1596	CD	PRO	1093	100.670	59.207	30.955	1.00	28.88
ATOM	1597	CA	PRO	1093	103.038	59.366	30.544	1.00	29.05
ATOM	1598	CB	PRO	1093	102.424	58.145	29.864	1.00	29.52
ATOM	1599	CG	PRO	1093	101.270	57.843	30.734	1.00	30.09
ATOM	1600	C	PRO	1093	103.807	60.199	29.532	1.00	29.67
ATOM	1601	O	PRO	1093	105.029	60.101	29.450	1.00	31.90
ATOM	1602	N	LYS	1094	103.081	61.014	28.767	1.00	29.17
ATOM	1603	CA	LYS	1094	103.669	61.855	27.729	1.00	28.35
ATOM	1604	CB	LYS	1094	102.769	61.857	26.492	1.00	25.80
ATOM	1605	CG	LYS	1094	102.678	60.505	25.833	1.00	26.73
ATOM	1606	CD	LYS	1094	102.036	60.568	24.467	1.00	28.73
ATOM	1607	CE	LYS	1094	102.138	59.217	23.790	1.00	30.21
ATOM	1608	NZ	LYS	1094	101.569	59.241	22.428	1.00	31.93

ATOM	1609	C	LYS	1094	103.934	63.281	28.177	1.00	29.51
ATOM	1610	O	LYS	1094	104.098	64.187	27.348	1.00	31.07
ATOM	1611	N	GLY	1095	104.021	63.471	29.487	1.00	30.06
ATOM	1612	CA	GLY	1095	104.261	64.794	30.035	1.00	29.06
ATOM	1613	C	GLY	1095	102.962	65.406	30.514	1.00	27.34
ATOM	1614	O	GLY	1095	101.935	64.724	30.527	1.00	28.11
ATOM	1615	N	PRO	1096	102.973	66.668	30.959	1.00	24.82
ATOM	1616	CD	PRO	1096	104.071	67.640	31.038	1.00	24.20
ATOM	1617	CA	PRO	1096	101.720	67.258	31.419	1.00	24.35
ATOM	1618	CB	PRO	1096	102.163	68.611	31.970	1.00	23.18
ATOM	1619	CG	PRO	1096	103.321	68.948	31.117	1.00	25.11
ATOM	1620	C	PRO	1096	100.732	67.401	30.268	1.00	24.48
ATOM	1621	O	PRO	1096	101.125	67.569	29.116	1.00	25.88
ATOM	1622	N	VAL	1097	99.450	67.270	30.582	1.00	25.45
ATOM	1623	CA	VAL	1097	98.393	67.386	29.595	1.00	24.09
ATOM	1624	CB	VAL	1097	97.598	66.077	29.520	1.00	22.86
ATOM	1625	CG1	VAL	1097	96.393	66.224	28.609	1.00	21.59
ATOM	1626	CG2	VAL	1097	98.510	64.964	29.009	1.00	23.88
ATOM	1627	C	VAL	1097	97.495	68.563	29.973	1.00	24.81
ATOM	1628	O	VAL	1097	97.051	68.675	31.113	1.00	25.35
ATOM	1629	N	ILE	1098	97.298	69.478	29.032	1.00	25.32
ATOM	1630	CA	ILE	1098	96.474	70.666	29.252	1.00	25.37
ATOM	1631	CB	ILE	1098	96.731	71.698	28.135	1.00	27.24
ATOM	1632	CG2	ILE	1098	96.029	73.015	28.447	1.00	26.41
ATOM	1633	CG1	ILE	1098	98.247	71.932	28.008	1.00	30.74
ATOM	1634	CD1	ILE	1098	98.659	72.943	26.946	1.00	32.59
ATOM	1635	C	ILE	1098	94.986	70.313	29.331	1.00	23.54
ATOM	1636	O	ILE	1098	94.546	69.325	28.752	1.00	24.20
ATOM	1637	N	GLN	1099	94.212	71.120	30.043	1.00	20.79
ATOM	1638	CA	GLN	1099	92.787	70.853	30.193	1.00	20.64
ATOM	1639	CB	GLN	1099	92.188	71.774	31.236	1.00	16.40
ATOM	1640	CG	GLN	1099	92.897	71.747	32.534	1.00	17.16
ATOM	1641	CD	GLN	1099	92.215	72.607	33.541	1.00	20.14
ATOM	1642	OE1	GLN	1099	91.129	73.118	33.286	1.00	25.87
ATOM	1643	NE2	GLN	1099	92.827	72.767	34.704	1.00	21.32
ATOM	1644	C	GLN	1099	91.973	70.990	28.918	1.00	22.84
ATOM	1645	O	GLN	1099	92.217	71.882	28.109	1.00	25.86
ATOM	1646	N	MET	1100	91.006	70.090	28.752	1.00	23.50
ATOM	1647	CA	MET	1100	90.099	70.094	27.606	1.00	22.12
ATOM	1648	CB	MET	1100	89.418	68.737	27.447	1.00	20.94
ATOM	1649	CG	MET	1100	90.052	67.816	26.450	1.00	22.51
ATOM	1650	SD	MET	1100	88.916	66.522	25.981	1.00	22.15
ATOM	1651	CE	MET	1100	88.786	65.731	27.470	1.00	23.27
ATOM	1652	C	MET	1100	89.002	71.124	27.819	1.00	23.05
ATOM	1653	O	MET	1100	88.581	71.801	26.879	1.00	24.71
ATOM	1654	N	TYR	1101	88.495	71.180	29.047	1.00	22.24
ATOM	1655	CA	TYR	1101	87.424	72.098	29.402	1.00	20.19
ATOM	1656	CB	TYR	1101	86.103	71.340	29.561	1.00	19.75
ATOM	1657	CG	TYR	1101	85.809	70.388	28.431	1.00	21.76
ATOM	1658	CD1	TYR	1101	86.004	69.022	28.582	1.00	20.14
ATOM	1659	CE1	TYR	1101	85.784	68.146	27.525	1.00	22.53

FIGURE 3 (CONT.)

ATOM	1660	CD2	TYR	1101	85.383	70.859	27.195	1.00	22.07
ATOM	1661	CE2	TYR	1101	85.161	69.998	26.137	1.00	21.98
ATOM	1662	CZ	TYR	1101	85.363	68.642	26.304	1.00	22.76
ATOM	1663	OH	TYR	1101	85.130	67.781	25.254	1.00	24.74
ATOM	1664	C	TYR	1101	87.750	72.764	30.716	1.00	21.21
ATOM	1665	O	TYR	1101	88.437	72.187	31.560	1.00	22.22
ATOM	1666	N	THR	1102	87.236	73.973	30.890	1.00	23.24
ATOM	1667	CA	THR	1102	87.424	74.741	32.111	1.00	24.37
ATOM	1668	CB	THR	1102	88.640	75.681	32.013	1.00	24.53
ATOM	1669	OG1	THR	1102	89.738	74.991	31.399	1.00	23.57
ATOM	1670	CG2	THR	1102	89.047	76.169	33.403	1.00	22.58
ATOM	1671	C	THR	1102	86.175	75.597	32.244	1.00	25.86
ATOM	1672	O	THR	1102	85.658	76.094	31.246	1.00	28.08
ATOM	1673	N	ASN	1103	85.668	75.740	33.460	1.00	26.20
ATOM	1674	CA	ASN	1103	84.480	76.547	33.700	1.00	25.78
ATOM	1675	CB	ASN	1103	83.213	75.752	33.372	1.00	26.82
ATOM	1676	CG	ASN	1103	81.947	76.585	33.511	1.00	28.67
ATOM	1677	OD1	ASN	1103	81.932	77.609	34.199	1.00	30.76
ATOM	1678	ND2	ASN	1103	80.871	76.135	32.882	1.00	27.57
ATOM	1679	C	ASN	1103	84.480	76.995	35.156	1.00	26.25
ATOM	1680	O	ASN	1103	83.832	76.391	36.006	1.00	27.25
ATOM	1681	N	VAL	1104	85.212	78.069	35.430	1.00	27.39
ATOM	1682	CA	VAL	1104	85.333	78.611	36.776	1.00	28.21
ATOM	1683	CB	VAL	1104	86.025	79.980	36.783	1.00	27.51
ATOM	1684	CG1	VAL	1104	86.316	80.397	38.205	1.00	28.55
ATOM	1685	CG2	VAL	1104	87.298	79.948	35.963	1.00	28.06
ATOM	1686	C	VAL	1104	83.978	78.796	37.419	1.00	30.54
ATOM	1687	O	VAL	1104	83.803	78.517	38.604	1.00	31.53
ATOM	1688	N	ASP	1105	83.022	79.260	36.626	1.00	33.66
ATOM	1689	CA	ASP	1105	81.677	79.503	37.117	1.00	36.82
ATOM	1690	CB	ASP	1105	80.788	80.061	36.001	1.00	41.34
ATOM	1691	CG	ASP	1105	81.192	81.457	35.573	1.00	45.36
ATOM	1692	OD1	ASP	1105	81.157	82.369	36.429	1.00	47.53
ATOM	1693	OD2	ASP	1105	81.543	81.636	34.382	1.00	48.54
ATOM	1694	C	ASP	1105	81.058	78.241	37.676	1.00	36.71
ATOM	1695	O	ASP	1105	80.645	78.200	38.835	1.00	36.88
ATOM	1696	N	GLN	1106	81.011	77.203	36.851	1.00	36.71
ATOM	1697	CA	GLN	1106	80.417	75.940	37.266	1.00	36.44
ATOM	1698	CB	GLN	1106	79.895	75.194	36.042	1.00	38.58
ATOM	1699	CG	GLN	1106	78.821	76.012	35.312	1.00	43.02
ATOM	1700	CD	GLN	1106	78.192	75.305	34.120	1.00	44.86
ATOM	1701	OE1	GLN	1106	77.334	75.870	33.437	1.00	44.11
ATOM	1702	NE2	GLN	1106	78.606	74.068	33.866	1.00	47.22
ATOM	1703	C	GLN	1106	81.342	75.077	38.122	1.00	34.06
ATOM	1704	O	GLN	1106	80.930	74.029	38.625	1.00	33.78
ATOM	1705	N	ASP	1107	82.561	75.575	38.339	1.00	29.82
ATOM	1706	CA	ASP	1107	83.577	74.900	39.144	1.00	26.00
ATOM	1707	CB	ASP	1107	83.039	74.635	40.551	1.00	26.29
ATOM	1708	CG	ASP	1107	84.138	74.436	41.574	1.00	25.28
ATOM	1709	OD1	ASP	1107	85.287	74.822	41.303	1.00	26.49
ATOM	1710	OD2	ASP	1107	83.844	73.914	42.666	1.00	25.48

FIGURE 3 (CONT.)

ATOM	1711	C	ASP	1107	84.016	73.597	38.492	1.00	23.82
ATOM	1712	O	ASP	1107	84.348	72.637	39.176	1.00	23.57
ATOM	1713	N	LEU	1108	84.066	73.593	37.167	1.00	21.98
ATOM	1714	CA	LEU	1108	84.440	72.413	36.403	1.00	22.63
ATOM	1715	CB	LEU	1108	83.349	72.083	35.378	1.00	21.22
ATOM	1716	CG	LEU	1108	82.093	71.415	35.928	1.00	21.50
ATOM	1717	CD1	LEU	1108	81.053	71.249	34.840	1.00	21.03
ATOM	1718	CD2	LEU	1108	82.473	70.079	36.506	1.00	20.86
ATOM	1719	C	LEU	1108	85.781	72.524	35.686	1.00	22.72
ATOM	1720	O	LEU	1108	86.206	73.608	35.285	1.00	24.88
ATOM	1721	N	VAL	1109	86.413	71.375	35.495	1.00	20.91
ATOM	1722	CA	VAL	1109	87.695	71.260	34.820	1.00	20.17
ATOM	1723	CB	VAL	1109	88.855	71.399	35.833	1.00	21.15
ATOM	1724	CG1	VAL	1109	90.117	70.788	35.292	1.00	22.22
ATOM	1725	CG2	VAL	1109	89.092	72.858	36.156	1.00	22.70
ATOM	1726	C	VAL	1109	87.674	69.850	34.245	1.00	19.05
ATOM	1727	O	VAL	1109	87.065	68.967	34.839	1.00	19.81
ATOM	1728	N	GLY	1110	88.306	69.648	33.092	1.00	17.18
ATOM	1729	CA	GLY	1110	88.328	68.334	32.477	1.00	16.06
ATOM	1730	C	GLY	1110	89.518	68.134	31.558	1.00	17.59
ATOM	1731	O	GLY	1110	89.896	69.050	30.823	1.00	16.16
ATOM	1732	N	TRP	1111	90.139	66.957	31.650	1.00	17.19
ATOM	1733	CA	TRP	1111	91.299	66.569	30.835	1.00	16.21
ATOM	1734	CB	TRP	1111	92.498	66.181	31.721	1.00	14.75
ATOM	1735	CG	TRP	1111	93.039	67.225	32.642	1.00	11.64
ATOM	1736	CD2	TRP	1111	92.802	67.337	34.058	1.00	11.04
ATOM	1737	CE2	TRP	1111	93.577	68.419	34.525	1.00	11.37
ATOM	1738	CE3	TRP	1111	92.011	66.626	34.973	1.00	13.68
ATOM	1739	CD1	TRP	1111	93.916	68.213	32.321	1.00	11.69
ATOM	1740	NE1	TRP	1111	94.247	68.935	33.447	1.00	14.19
ATOM	1741	CZ2	TRP	1111	93.589	68.809	35.867	1.00	11.96
ATOM	1742	CZ3	TRP	1111	92.022	67.011	36.308	1.00	11.51
ATOM	1743	CH2	TRP	1111	92.808	68.095	36.741	1.00	13.13
ATOM	1744	C	TRP	1111	90.873	65.290	30.125	1.00	17.82
ATOM	1745	O	TRP	1111	89.882	64.670	30.516	1.00	20.28
ATOM	1746	N	PRO	1112	91.581	64.885	29.053	1.00	18.22
ATOM	1747	CD	PRO	1112	92.711	65.493	28.331	1.00	17.52
ATOM	1748	CA	PRO	1112	91.153	63.637	28.406	1.00	16.49
ATOM	1749	CB	PRO	1112	92.189	63.452	27.309	1.00	15.54
ATOM	1750	CG	PRO	1112	92.586	64.846	26.978	1.00	18.88
ATOM	1751	C	PRO	1112	91.318	62.567	29.477	1.00	18.48
ATOM	1752	O	PRO	1112	92.207	62.679	30.322	1.00	21.84
ATOM	1753	N	ALA	1113	90.443	61.573	29.512	1.00	19.42
ATOM	1754	CA	ALA	1113	90.572	60.540	30.526	1.00	18.50
ATOM	1755	CB	ALA	1113	89.441	59.543	30.420	1.00	17.46
ATOM	1756	C	ALA	1113	91.909	59.851	30.319	1.00	20.35
ATOM	1757	O	ALA	1113	92.278	59.532	29.189	1.00	21.19
ATOM	1758	N	PRO	1114	92.689	59.681	31.396	1.00·	21.47
ATOM	1759	CD	PRO	1114	92.488	60.128	32.783	1.00	22.45
ATOM	1760	CA	PRO	1114	93.984	59.022	31.250	1.00	22.96
ATOM	1761	CB	PRO	1114	94.529	59.018	32.682	1.00	23.65

FIGURE 3 (CONT.)

ATOM	1762	CG	PRO	1114	93.306	59.138	33.537	1.00	22.54
ATOM	1763	C	PRO	1114	93.835	57.620	30.693	1.00	24.51
ATOM	1764	O	PRO	1114	92.888	56.903	31.024	1.00	26.99
ATOM	1765	N	GLN	1115	94.730	57.254	29.786	1.00	26.09
ATOM	1766	CA	GLN	1115	94.706	55.925	29.195	1.00	28.46
ATOM	1767	CB	GLN	1115	95.903	55.744	28.258	1.00	30.59
ATOM	1768	CG	GLN	1115	95.895	56.656	27.033	1.00	34.32
ATOM	1769	CD	GLN	1115	94.865	56.236	26.009	1.00	37.60
ATOM	1770	OE1	GLN	1115	94.731	55.051	25.699	1.00	39.96
ATOM	1771	NE2	GLN	1115	94.122	57.203	25.479	1.00	41.37
ATOM	1772	C	GLN	1115	94.762	54.895	30.325	1.00	28.93
ATOM	1773	O	GLN	1115	95.548	55.039	31.269	1.00	29.99
ATOM	1774	N	GLY	1116	93.881	53.902	30.257	1.00	28.45
ATOM	1775	CA	GLY	1116	93.842	52.862	31.272	1.00	28.19
ATOM	1776	C	GLY	1116	92.595	52.883	32.140	1.00	28.90
ATOM	1777	O	GLY	1116	92.155	51.840	32.633	1.00	30.64
ATOM	1778	N	SER	1117	92.027	54.071	32.327	1.00	28.03
ATOM	1779	CA	SER	1117	90.834	54.246	33.143	1.00	25.22
ATOM	1780	CB	SER	1117	90.688	55.717	33.517	1.00	21.89
ATOM	1781	OG	SER	1117	90.524	56.491	32.349	1.00	17.60
ATOM	1782	C	SER	1117	89.567	53.784	32.432	1.00	25.37
ATOM	1783	O	SER	1117	89.592	53.456	31.241	1.00	26.03
ATOM	1784	N	ARG	1118	88.468	53.734	33.181	1.00	25.35
ATOM	1785	CA	ARG	1118	87.170	53.350	32.641	1.00	25.91
ATOM	1786	CB	ARG	1118	86.635	52.074	33.300	1.00	31.51
ATOM	1787	CG	ARG	1118	87.368	50.796	32.919	1.00	42.46
ATOM	1788	CD	ARG	1118	87.604	50.721	31.414	1.00	51.80
ATOM	1789	NE	ARG	1118	87.874	49.357	30.956	1.00	61.09
ATOM	1790	CZ	ARG	1118	88.830	49.022	30.090	1.00	65.33
ATOM	1791	NH1	ARG	1118	88.981	47.749	29.738	1.00	68.07
ATOM	1792	NH2	ARG	1118	89.661	49.941	29.606	1.00	67.27
ATOM	1793	C	ARG	1118	86.252	54.515	32.960	1.00	24.68
ATOM	1794	O	ARG	1118	86.375	55.128	34.020	1.00	24.68
ATOM	1795	N	SER	1119	85.355	54.844	32.043	1.00	22.26
ATOM	1796	CA	SER	1119	84.446	55.957	32.263	1.00	22.87
ATOM	1797	CB	SER	1119	84.333	56.807	30.993	1.00	21.77
ATOM	1798	OG	SER	1119	85.535	57.511	30.735	1.00	26.02
ATOM	1799	C	SER	1119	83.053	55.536	32.692	1.00	20.90
ATOM	1800	O	SER	1119	82.620	54.421	32.425	1.00	21.97
ATOM	1801	N	LEU	1120	82.379	56.424	33.409	1.00	19.67
ATOM	1802	CA	LEU	1120	81.008	56.195	33.827	1.00	16.91
ATOM	1803	CB	LEU	1120	80.691	56.939	35.131	1.00	13.88
ATOM	1804	CG	LEU	1120	81.329	56.564	36.469	1.00	11.68
ATOM	1805	CD1	LEU	1120	80.978	57.623	37.470	1.00	11.76
ATOM	1806	CD2	LEU	1120	80.854	55.209	36.950	1.00	13.04
ATOM	1807	C	LEU	1120	80.197	56.828	32.704	1.00	16.42
ATOM	1808	O	LEU	1120	80.753	57.509	31.840	1.00	15.05
ATOM	1809	N	THR	1121	78.893	56.602	32.714	1.00	18.09
ATOM	1810	CA	THR	1121	78.012	57.189	31.719	1.00	19.50
ATOM	1811	CB	THR	1121	77.383	56.120	30.825	1.00	20.88
ATOM	1812	OG1	THR	1121	77.011	54.987	31.620	1.00	26.65

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FIGURE 3 (CONT.)

ATOM	1813	CG2	THR	1121	78.372	55.683	29.758	1.00	21.77
ATOM	1814	C	THR	1121	76.938	57.941	32.485	1.00	18.52
ATOM	1815	O	THR	1121	76.613	57.579	33.616	1.00	20.72
ATOM	1816	N	PRO	1122	76.441	59.052	31.931	1.00	18.23
ATOM	1817	CD	PRO	1122	76.865	59.703	30.680	1.00	17.02
ATOM	1818	CA	PRO	1122	75.403	59.835	32.606	1.00	18.29
ATOM	1819	CB	PRO	1122	75.108	60.939	31.600	1.00	18.11
ATOM	1820	CG	PRO	1122	76.432	61.122	30.908	1.00	16.83
ATOM	1821	C	PRO	1122	74.153	59.019	32.931	1.00	20.74
ATOM	1822	O	PRO	1122	73.887	57.985	32.317	1.00	22.14
ATOM	1823	N	CYS	1123	73.405	59.476	33.925	1.00	23.09
ATOM	1824	CA	CYS	1123	72.184	58.807	34.348	1.00	25.58
ATOM	1825	CB	CYS	1123	71.811	59.265	35.759	1.00	25.03
ATOM	1826	SG	CYS	1123	70.363	58.469	36.474	1.00	22.23
ATOM	1827	C	CYS	1123	71.069	59.169	33.381	1.00	27.87
ATOM	1828	O	CYS	1123	70.978	60.314	32.942	1.00	29.71
ATOM	1829	N	THR	1124	70.211	58.199	33.075	1.00	30.25
ATOM	1830	CA	THR	1124	69.086	58.398	32.162	1.00	30.66
ATOM	1831	CB	THR	1124	69.407	57.845	30.756	1.00	29.19
ATOM	1832	OG1	THR	1124	69.987	56.537	30.874	1.00	28.07
ATOM	1833	CG2	THR	1124	70.354	58.776	30.009	1.00	26.85
ATOM	1834	C	THR	1124	67.853	57.684	32.720	1.00	32.73
ATOM	1835	O	THR	1124	67.224	56.867	32.049	1.00	35.79
ATOM	1836	N	CYS	1125	67.532	57.980	33.971	1.00	33.01
ATOM	1837	CA	CYS	1125	66.395	57.373	34.639	1.00	32.02
ATOM	1838	CB	CYS	1125	66.836	56.136	35.433	1.00	33.60
ATOM	1839	SG	CYS	1125	67.885	56.458	36.910	1.00	37.33
ATOM	1840	C	CYS	1125	65.785	58.403	35.571	1.00	31.70
ATOM	1841	O	CYS	1125	64.771	58.151	36.211	1.00	35.06
ATOM	1842	N	GLY	1126	66.417	59.569	35.642	1.00	30.53
ATOM	1843	CA	GLY	1126	65.927	60.636	36.490	1.00	30.87
ATOM	1844	C	GLY	1126	65.769	60.278	37.954	1.00	30.72
ATOM	1845	O	GLY	1126	65.092	60.991	38.691	1.00	33.42
ATOM	1846	N	SER	1127	66.408	59.200	38.394	1.00	29.86
ATOM	1847	CA	SER	1127	66.297	58.790	39.786	1.00	29.79
ATOM	1848	CB	SER	1127	67.098	57.519	40.045	1.00	28.49
ATOM	1849	OG	SER	1127	67.027	57.174	41.421	1.00	30.28
ATOM	1850	C	SER	1127	66.718	59.881	40.771	1.00	31.88
ATOM	1851	O	SER	1127	67.629	60.673	40.499	1.00	31.79
ATOM	1852	N	SER	1128	66.045	59.908	41.917	1.00	32.25
ATOM	1853	CA	SER	1128	66.335	60.884	42.957	1.00	32.78
ATOM	1854	CB	SER	1128	65.045	61.545	43.431	1.00	34.11
ATOM	1855	OG	SER	1128	64.117	60.564	43.869	1.00	38.32
ATOM	1856	C	SER	1128	67.061	60.246	44.139	1.00	31.47
ATOM	1857	O	SER	1128	67.345	60.924	45.130	1.00	30.85
ATOM	1858	N	ASP	1129	67.293	58.936	44.066	1.00	29.87
ATOM	1859	CA	ASP	1129	68.012	58.219	45.123	1.00	29.89
ATOM	1860	CB	ASP	1129	67.408	56.839	45.348	1.00	31.52
ATOM	1861	CG	ASP	1129	65.931	56.898	45.658	1.00	34.71
ATOM	1862	OD1	ASP	1129	65.561	57.534	46.667	1.00	36.72
ATOM	1863	OD2	ASP	1129	65.141	56.320	44.878	1.00	35.48

ATOM	1864	C	ASP	1129	69.442	58.075	44.624	1.00	29.13
ATOM	1865	O	ASP	1129	69.711	57.254	43.745	1.00	28.49
ATOM	1866	N	LEU	1130	70.342	58.886	45.177	1.00	27.18
ATOM	1867	CA	LEU	1130	71.740	58.907	44.760	1.00	24.28
ATOM	1868	CB	LEU	1130	72.156	60.349	44.445	1.00	23.07
ATOM	1869	CG	LEU	1130	71.172	61.255	43.689	1.00	21.59
ATOM	1870	CD1	LEU	1130	71.727	62.664	43.589	1.00	19.14
ATOM	1871	CD2	LEU	1130	70.883	60.693	42.319	1.00	19.32
ATOM	1872	C	LEU	1130	72.690	58.324	45.802	1.00	23.34
ATOM	1873	O	LEU	1130	72.347	58.198	46.979	1.00	24.14
ATOM	1874	N	TYR	1131	73.898	57.988	45.360	1.00	23.40
ATOM	1875	CA	TYR	1131	74.928	57.423	46.225	1.00	22.86
ATOM	1876	CB	TYR	1131	75.039	55.924	45.980	1.00	22.51
ATOM	1877	CG	TYR	1131	73.719	55.224	46.135	1.00	21.96
ATOM	1878	CD1	TYR	1131	72.923	54.955	45.034	1.00	21.81
ATOM	1879	CE1	TYR	1131	71.671	54.382	45.176	1.00	22.83
ATOM	1880	CD2	TYR	1131	73.234	54.893	47.393	1.00	24.12
ATOM	1881	CE2	TYR	1131	71.985	54.318	47.551	1.00	24.94
ATOM	1882	CZ	TYR	1131	71.205	54.065	46.437	1.00	24.69
ATOM	1883	OH	TYR	1131	69.951	53.504	46.590	1.00	26.44
ATOM	1884	C	TYR	1131	76.268	58.108	45.965	1.00	22.03
ATOM	1885	O	TYR	1131	76.773	58.088	44.847	1.00	22.92
ATOM	1886	N	LEU	1132	76.809	58.737	47.003	1.00	21.21
ATOM	1887	CA	LEU	1132	78.071	59.463	46.956	1.00	20.60
ATOM	1888	CB	LEU	1132	78.032	60.576	48.007	1.00	21.28
ATOM	1889	CG	LEU	1132	78.843	61.874	47.906	1.00	23.35
ATOM	1890	CD1	LEU	1132	78.614	62.661	49.172	1.00	25.61
ATOM	1891	CD2	LEU	1132	80.319	61.623	47.741	1.00	26.41
ATOM	1892	C	LEU	1132	79.249	58.541	47.263	1.00	20.51
ATOM	1893	O	LEU	1132	79.250	57.853	48.283	1.00	23.83
ATOM	1894	N	VAL	1133	80.246	58.524	46.386	1.00	18.28
ATOM	1895	CA	VAL	1133	81.438	57.714	46.592	1.00	16.12
ATOM	1896	CB	VAL	1133	81.912	57.067	45.284	1.00	14.27
ATOM	1897	CG1	VAL	1133	83.198	56.291	45.516	1.00	11.21
ATOM	1898	CG2	VAL	1133	80.821	56.165	44.722	1.00	9.93
ATOM	1899	C	VAL	1133	82.538	58.635	47.130	1.00	20.05
ATOM	1900	O	VAL	1133	83.051	59.504	46.411	1.00	18.89
ATOM	1901	N	THR	1134	82.861	58.471	48.410	1.00	21.68
ATOM	1902	CA	THR	1134	83.876	59.286	49.061	1.00	21.80
ATOM	1903	CB	THR	1134	83.741	59.227	50.584	1.00	19.89
ATOM	1904	OG1	THR	1134	84.183	57.946	51.043	1.00	21.40
ATOM	1905	CG2	THR	1134	82.292	59.428	50.999	1.00	18.10
ATOM	1906	C	THR	1134	85.296	58.872	48.705	1.00	24.10
ATOM	1907	O	THR	1134	85.530	57.792	48.166	1.00	24.71
ATOM	1908	N	ARG	1135	86.245	59.719	49.083	1.00	26.05
ATOM	1909	CA	ARG	1135	87.665	59.488	48.840	1.00	28.72
ATOM	1910	CB	ARG	1135	88.472	60.667	49.386	1.00	32.63
ATOM	1911	CG	ARG	1135	89.950	60.546	49.160	1.00	35.08
ATOM	1912	CD	ARG	1135	90.705	61.556	49.968	1.00	39.19
ATOM	1913	NE	ARG	1135	92.134	61.292	49.896	1.00	46.35
ATOM	1914	CZ	ARG	1135	93.018	61.704	50.798	1.00	53.28

FIGURE 3 (CONT.)

ATOM	1915	NH1	ARG	1135	94.305	61.414	50.643	1.00	56.95
ATOM	1916	NH2	ARG	1135	92.618	62.396	51.862	1.00	57.23
ATOM	1917	C	ARG	1135	88.173	58.202	49.487	1.00	27.12
ATOM	1918	O	ARG	1135	89.205	57.668	49.094	1.00	28.70
ATOM	1919	N	HIS	1136	87.471	57.732	50.508	1.00	26.02
ATOM	1920	CA	HIS	1136	87.875	56.517	51.201	1.00	25.17
ATOM	1921	CB	HIS	1136	87.613	56.649	52.695	1.00	27.11
ATOM	1922	CG	HIS	1136	88.126	57.929	53.272	1.00	33.56
ATOM	1923	CD2	HIS	1136	87.473	59.032	53.704	1.00	37.55
ATOM	1924	ND1	HIS	1136	89.473	58.206	53.392	1.00	35.53
ATOM	1925	CE1	HIS	1136	89.626	59.429	53.869	1.00	38.38
ATOM	1926	NE2	HIS	1136	88.429	59.954	54.068	1.00	39.18
ATOM	1927	C	HIS	1136	87.150	55.306	50.645	1.00	24.36
ATOM	1928	O	HIS	1136	87.172	54.236	51.252	1.00	24.55
ATOM	1929	N	ALA	1137	86.522	55.480	49.485	1.00	21.92
ATOM	1930	CA	ALA	1137	85.796	54.413	48.823	1.00	20.47
ATOM	1931	CB	ALA	1137	86.728	53.257	48.511	1.00	20.48
ATOM	1932	C	ALA	1137	84.588	53.934	49.623	1.00	21.30
ATOM	1933	O	ALA	1137	84.316	52.734	49.719	1.00	22.24
ATOM	1934	N	ASP	1138	83.876	54.880	50.218	1.00	21.09
ATOM	1935	CA	ASP	1138	82.674	54.569	50.973	1.00	21.30
ATOM	1936	CB	ASP	1138	82.662	55.283	52.325	1.00	20.40
ATOM	1937	CG	ASP	1138	83.685	54.731	53.291	1.00	20.82
ATOM	1938	OD1	ASP	1138	83.890	53.501	53.319	1.00	23.51
ATOM	1939	OD2	ASP	1138	84.287	55.527	54.034	1.00	23.93
ATOM	1940	C	ASP	1138	81.537	55.097	50.119	1.00	23.33
ATOM	1941	O	ASP	1138	81.646	56.183	49.546	1.00	25.82
ATOM	1942	N	VAL	1139	80.468	54.320	50.003	1.00	23.72
ATOM	1943	CA	VAL	1139	79.305	54.702	49.214	1.00	20.95
ATOM	1944	CB	VAL	1139	78.779	53.501	48.415	1.00	18.28
ATOM	1945	CG1	VAL	1139	77.527	53.875	47.661	1.00	15.80
ATOM	1946	CG2	VAL	1139	79.857	52.982	47.481	1.00	12.00
ATOM	1947	C	VAL	1139	78.251	55.125	50.208	1.00	22.42
ATOM	1948	O	VAL	1139	77.814	54.316	51.017	1.00	25.81
ATOM	1949	N	ILE	1140	77.862	56.389	50.188	1.00	23.66
ATOM	1950	CA	ILE	1140	76.854	56.863	51.130	1.00	25.17
ATOM	1951	CB	ILE	1140	77.449	57.935	52.089	1.00	26.79
ATOM	1952	CG2	ILE	1140	78.669	57.368	52.805	1.00	27.35
ATOM	1953	CG1	ILE	1140	77.887	59.188	51.330	1.00	28.07
ATOM	1954	CD1	ILE	1140	78.560	60.238	52.219	1.00	27.71
ATOM	1955	C	ILE	1140	75.607	57.375	50.408	1.00	25.17
ATOM	1956	O	ILE	1140	75.717	58.102	49.433	1.00	25.94
ATOM	1957	N	PRO	1141	74.406	56.943	50.834	1.00	25.23
ATOM	1958	CD	PRO	1141	74.102	56.065	51.974	1.00	26.31
ATOM	1959	CA	PRO	1141	73.167	57.388	50.189	1.00	26.02
ATOM	1960	CB	PRO	1141	72.099	56.552	50.887	1.00	26.05
ATOM	1961	CG	PRO	1141	72.647	56.404	52.253	1.00	26.71
ATOM	1962	C	PRO	1141	72.912	58.874	50.384	1.00	27.84
ATOM	1963	O	PRO	1141	73.231	59.440	51.432	1.00	29.15
ATOM	1964	N	VAL	1142	72.289	59.483	49.383	1.00	28.51
ATOM	1965	CA	VAL	1142	71.973	60.902	49.385	1.00	27.59

FIGURE 3 (CONT.)

ATOM	1966	CB	VAL	1142	73.080	61.695	48.640	1.00	26.82
ATOM	1967	CG1	VAL	1142	72.710	63.160	48.504	1.00	25.54
ATOM	1968	CG2	VAL	1142	74.398	61.554	49.368	1.00	24.22
ATOM	1969	C	VAL	1142	70.650	61.047	48.640	1.00	30.42
ATOM	1970	O	VAL	1142	70.465	60.445	47.575	1.00	31.72
ATOM	1971	N	ARG	1143	69.708	61.788	49.220	1.00	32.81
ATOM	1972	CA	ARG	1143	68.411	62.006	48.580	1.00	33.55
ATOM	1973	CB	ARG	1143	67.282	62.037	49.613	1.00	35.71
ATOM	1974	CG	ARG	1143	65.903	62.331	49.017	1.00	37.69
ATOM	1975	CD	ARG	1143	65.465	61.288	47.991	1.00	39.30
ATOM	1976	NE	ARG	1143	64.225	61.685	47.311	1.00	43.20
ATOM	1977	CZ	ARG	1143	63.383	60.843	46.711	1.00	43.40
ATOM	1978	NH1	ARG	1143	63.628	59.539	46.696	1.00	43.88
ATOM	1979	NH2	ARG	1143	62.297	61.307	46.108	1.00	43.09
ATOM	1980	C	ARG	1143	68.439	63.320	47.818	1.00	33.27
ATOM	1981	O	ARG	1143	68.794	64.353	48.382	1.00	33.50
ATOM	1982	N	ARG	1144	68.044	63.280	46.549	1.00	33.18
ATOM	1983	CA	ARG	1144	68.038	64.471	45.709	1.00	34.20
ATOM	1984	CB	ARG	1144	67.725	64.089	44.260	1.00	32.94
ATOM	1985	CG	ARG	1144	68.475	64.900	43.203	1.00	32.47
ATOM	1986	CD	ARG	1144	67.952	64.546	41.815	1.00	32.92
ATOM	1987	NE	ARG	1144	68.924	64.732	40.738	1.00	33.75
ATOM	1988	CZ	ARG	1144	69.459	65.898	40.387	1.00	35.07
ATOM	1989	NH1	ARG	1144	69.125	67.007	41.029	1.00	36.60
ATOM	1990	NH2	ARG	1144	70.321	65.959	39.378	1.00	35.64
ATOM	1991	C	ARG	1144	67.001	65.467	46.227	1.00	35.48
ATOM	1992	O	ARG	1144	65.825	65.139	46.374	1.00	36.95
ATOM	1993	N	ARG	1145	67.449	66.670	46.546	1.00	36.40
ATOM	1994	CA	ARG	1145	66.552	67.700	47.048	1.00	37.95
ATOM	1995	CB	ARG	1145	67.025	68.213	48.414	1.00	37.18
ATOM	1996	CG	ARG	1145	66.975	67.184	49.514	1.00	36.94
ATOM	1997	CD	ARG	1145	65.570	66.667	49.681	1.00	38.43
ATOM	1998	NE	ARG	1145	65.447	65.729	50.791	1.00	41.86
ATOM	1999	CZ	ARG	1145	64.341	65.043	51.062	1.00	43.83
ATOM	2000	NH1	ARG	1145	63.263	65.187	50.299	1.00	46.04
ATOM	2001	NH2	ARG	1145	64.306	64.223	52.102	1.00	45.68
ATOM	2002	C	ARG	1145	66.507	68.856	46.063	1.00	39.67
ATOM	2003	O	ARG	1145	66.247	70.000	46.449	1.00	42.26
ATOM	2004	N	GLY	1146	66.789	68.565	44.797	1.00	39.96
ATOM	2005	CA	GLY	1146	66.779	69.605	43.788	1.00	40.13
ATOM	2006	C	GLY	1146	67.932	69.428	42.823	1.00	40.68
ATOM	2007	O	GLY	1146	68.829	68.621	43.061	1.00	41.79
ATOM	2008	N	ALA	1147	67.937	70.228	41.765	1.00	40.55
ATOM	2009	CA	ALA	1147	68.961	70.157	40.733	1.00	39.49
ATOM	2010	CB	ALA	1147	68.890	71.392	39.834	1.00	40.92
ATOM	2011	C	ALA	1147	70.392	69.927	41.214	1.00	38.50
ATOM	2012	O	ALA	1147	71.068	69.024	40.717	1.00	38.36
ATOM	2013	N	SER	1148	70.854	70.721	42.176	1.00	37.84
ATOM	2014	CA	SER	1148	72.222	70.564	42.656	1.00	36.96
ATOM	2015	CB	SER	1148	73.097	71.732	42.182	1.00	36.77
ATOM	2016	OG	SER	1148	72.690	72.965	42.755	1.00	40.56

FIGURE 3 (CONT.)

ATOM	2017	C	SER	1148	72.391	70.363	44.156	1.00	36.04
ATOM	2018	O	SER	1148	73.382	70.812	44.734	1.00	36.47
ATOM	2019	N	ARG	1149	71.452	69.672	44.788	1.00	34.56
ATOM	2020	CA	ARG	1149	71.575	69.416	46.214	1.00	33.98
ATOM	2021	CB	ARG	1149	70.923	70.518	47.050	1.00	35.91
ATOM	2022	CG	ARG	1149	71.621	70.740	48.397	1.00	40.83
ATOM	2023	CD	ARG	1149	70.760	71.514	49.389	1.00	44.70
ATOM	2024	NE	ARG	1149	71.544	72.142	50.456	1.00	48.33
ATOM	2025	CZ	ARG	1149	71.832	73.444	50.506	1.00	50.37
ATOM	2026	NH1	ARG	1149	71.416	74.266	49.552	1.00	52.98
ATOM	2027	NH2	ARG	1149	72.508	73.941	51.531	1.00	51.44
ATOM	2028	C	ARG	1149	70.981	68.070	46.573	1.00	32.53
ATOM	2029	O	ARG	1149	70.168	67.513	45.833	1.00	32.88
ATOM	2030	N	GLY	1150	71.418	67.541	47.705	1.00	31.86
ATOM	2031	CA	GLY	1150	70.934	66.260	48.171	1.00	29.91
ATOM	2032	C	GLY	1150	71.207	66.138	49.653	1.00	28.10
ATOM	2033	O	GLY	1150	72.237	66.603	50.137	1.00	29.55
ATOM	2034	N	SER	1151	70.289	65.516	50.376	1.00	27.99
ATOM	2035	CA	SER	1151	70.439	65.348	51.811	1.00	28.25
ATOM	2036	CB	SER	1151	69.072	65.434	52.487	1.00	31.79
ATOM	2037	OG	SER	1151	68.433	66.664	52.201	1.00	39.70
ATOM	2038	C	SER	1151	71.071	64.020	52.164	1.00	26.53
ATOM	2039	O	SER	1151	70.653	62.974	51.662	1.00	25.17
ATOM	2040	N	LEU	1152	72.089	64.055	53.013	1.00	25.87
ATOM	2041	CA	LEU	1152	72.706	62.814	53.443	1.00	27.78
ATOM	2042	CB	LEU	1152	73.948	63.075	54.296	1.00	26.21
ATOM	2043	CG	LEU	1152	75.157	63.729	53.627	1.00	24.51
ATOM	2044	CD1	LEU	1152	76.335	63.659	54.564	1.00	23.77
ATOM	2045	CD2	LEU	1152	75.496	63.008	52.343	1.00	25.98
ATOM	2046	C	LEU	1152	71.629	62.147	54.287	1.00	29.68
ATOM	2047	O	LEU	1152	70.965	62.819	55.075	1.00	31.97
ATOM	2048	N	LEU	1153	71.385	60.860	54.065	1.00	31.23
ATOM	2049	CA	LEU	1153	70.372	60.159	54.845	1.00	31.26
ATOM	2050	CB	LEU	1153	69.991	58.836	54.181	1.00	29.73
ATOM	2051	CG	LEU	1153	68.811	58.932	53.215	1.00	27.81
ATOM	2052	CD1	LEU	1153	69.023	60.036	52.193	1.00	29.89
ATOM	2053	CD2	LEU	1153	68.619	57.614	52.528	1.00	28.98
ATOM	2054	C	LEU	1153	70.862	59.933	56.269	1.00	33.19
ATOM	2055	O	LEU	1153	70.075	59.670	57.182	1.00	34.12
ATOM	2056	N	SER	1154	72.166	60.072	56.459	1.00	34.74
ATOM	2057	CA	SER	1154	72.775	59.899	57.762	1.00	37.99
ATOM	2058	CB	SER	1154	73.331	58.483	57.903	1.00	40.16
ATOM	2059	OG	SER	1154	72.446	57.531	57.326	1.00	44.40
ATOM	2060	C	SER	1154	73.910	60.907	57.871	1.00	38.37
ATOM	2061	O	SER	1154	74.946	60.743	57.236	1.00	38.18
ATOM	2062	N	PRO	1155	73.694	62.005	58.622	1.00	38.99
ATOM	2063	CD	PRO	1155	72.505	62.296	59.437	1.00	39.19
ATOM	2064	CA	PRO	1155	74.708	63.045	58.805	1.00	38.38
ATOM	2065	CB	PRO	1155	74.098	63.942	59.875	1.00	38.04
ATOM	2066	CG	PRO	1155	73.120	63.040	60.584	1.00	40.36
ATOM	2067	C	PRO	1155	76.048	62.479	59.245	1.00	37.35

FIGURE 3 (CONT.)

ATOM	2068	O	PRO	1155	76.121	61.531	60.044	1.00	36.59
ATOM	2069	N	ARG	1156	77.104	63.088	58.732	1.00	36.29
ATOM	2070	CA	ARG	1156	78.456	62.654	59.023	1.00	35.23
ATOM	2071	CB	ARG	1156	79.031	61.956	57.803	1.00	38.13
ATOM	2072	CG	ARG	1156	78.185	60.870	57.211	1.00	41.38
ATOM	2073	CD	ARG	1156	78.700	59.509	57.644	1.00	44.77
ATOM	2074	NE	ARG	1156	78.123	58.412	56.868	1.00	49.49
ATOM	2075	CZ	ARG	1156	78.459	57.129	57.005	1.00	53.79
ATOM	2076	NH1	ARG	1156	77.873	56.205	56.252	1.00	54.43
ATOM	2077	NH2	ARG	1156	79.403	56.763	57.863	1.00	52.82
ATOM	2078	C	ARG	1156	79.340	63.849	59.255	1.00	34.55
ATOM	2079	O	ARG	1156	79.066	64.939	58.756	1.00	35.72
ATOM	2080	N	PRO	1157	80.443	63.673	59.989	1.00	34.18
ATOM	2081	CD	PRO	1157	80.899	62.473	60.707	1.00	33.27
ATOM	2082	CA	PRO	1157	81.344	64.798	60.233	1.00	33.99
ATOM	2083	CB	PRO	1157	82.419	64.167	61.111	1.00	33.27
ATOM	2084	CG	PRO	1157	81.690	63.074	61.803	1.00	32.25
ATOM	2085	C	PRO	1157	81.950	65.234	58.898	1.00	35.59
ATOM	2086	O	PRO	1157	82.404	64.393	58.130	1.00	37.92
ATOM	2087	N	ILE	1158	81.999	66.527	58.631	1.00	36.57
ATOM	2088	CA	ILE	1158	82.542	67.000	57.362	1.00	38.10
ATOM	2089	CB	ILE	1158	82.647	68.533	57.315	1.00	38.12
ATOM	2090	CG2	ILE	1158	81.272	69.140	57.171	1.00	37.34
ATOM	2091	CG1	ILE	1158	83.342	69.046	58.573	1.00	41.61
ATOM	2092	CD1	ILE	1158	83.623	70.540	58.559	1.00	45.60
ATOM	2093	C	ILE	1158	83.911	66.408	57.004	1.00	39.96
ATOM	2094	O	ILE	1158	84.280	66.367	55.828	1.00	41.17
ATOM	2095	N	SER	1159	84.642	65.941	58.014	1.00	40.39
ATOM	2096	CA	SER	1159	85.959	65.341	57.813	1.00	42.66
ATOM	2097	CB	SER	1159	86.575	64.975	59.161	1.00	45.98
ATOM	2098	OG	SER	1159	85.755	64.035	59.842	1.00	49.77
ATOM	2099	C	SER	1159	85.870	64.078	56.955	1.00	42.30
ATOM	2100	O	SER	1159	86.779	63.761	56.183	1.00	43.56
ATOM	2101	N	TYR	1160	84.779	63.346	57.130	1.00	40.66
ATOM	2102	CA	TYR	1160	84.531	62.121	56.385	1.00	40.36
ATOM	2103	CB	TYR	1160	83.137	61.598	56.756	1.00	43.66
ATOM	2104	CG	TYR	1160	82.848	60.149	56.423	1.00	47.75
ATOM	2105	CD1	TYR	1160	82.086	59.377	57.290	1.00	50.46
ATOM	2106	CE1	TYR	1160	81.763	58.059	56.991	1.00	53.68
ATOM	2107	CD2	TYR	1160	83.293	59.561	55.233	1.00	49.34
ATOM	2108	CE2	TYR	1160	82.975	58.237	54.922	1.00	51.68
ATOM	2109	CZ	TYR	1160	82.205	57.493	55.809	1.00	53.15
ATOM	2110	OH	TYR	1160	81.858	56.185	55.528	1.00	54.20
ATOM	2111	C	TYR	1160	84.563	62.464	54.901	1.00	37.91
ATOM	2112	O	TYR	1160	85.111	61.715	54.080	1.00	38.62
ATOM	2113	N	LEU	1161	84.020	63.632	54.578	1.00	34.26
ATOM	2114	CA	LEU	1161	83.932	64.086	53.203	1.00	30.68
ATOM	2115	CB	LEU	1161	82.639	64.889	53.018	1.00	27.49
ATOM	2116	CG	LEU	1161	81.344	64.152	53.394	1.00	25.85
ATOM	2117	CD1	LEU	1161	80.168	65.085	53.276	1.00	25.64
ATOM	2118	CD2	LEU	1161	81.135	62.931	52.516	1.00	23.54

FIGURE 3 (CONT.)

ATOM	2119	C	LEU	1161	85.148	64.852	52.675	1.00	30.40
ATOM	2120	O	LEU	1161	85.242	65.106	51.473	1.00	31.18
ATOM	2121	N	ALA	1162	86.094	65.189	53.545	1.00	29.45
ATOM	2122	CA	ALA	1162	87.283	65.919	53.101	1.00	29.15
ATOM	2123	CB	ALA	1162	88.222	66.214	54.281	1.00	29.64
ATOM	2124	C	ALA	1162	88.024	65.140	52.015	1.00	27.83
ATOM	2125	O	ALA	1162	88.278	63.937	52.150	1.00	28.97
ATOM	2126	N	GLY	1163	88.324	65.830	50.922	1.00	26.09
ATOM	2127	CA	GLY	1163	89.032	65.216	49.816	1.00	24.79
ATOM	2128	C	GLY	1163	88.127	64.490	48.845	1.00	22.40
ATOM	2129	O	GLY	1163	88.607	63.799	47.958	1.00	22.88
ATOM	2130	N	SER	1164	86.819	64.667	48.978	1.00	23.08
ATOM	2131	CA	SER	1164	85.887	63.988	48.091	1.00	23.47
ATOM	2132	CB	SER	1164	84.765	63.336	48.893	1.00	22.44
ATOM	2133	OG	SER	1164	85.308	62.418	49.833	1.00	24.67
ATOM	2134	C	SER	1164	85.314	64.853	46.984	1.00	23.93
ATOM	2135	O	SER	1164	84.470	64.389	46.229	1.00	25.83
ATOM	2136	N	SER	1165	85.762	66.102	46.877	1.00	24.65
ATOM	2137	CA	SER	1165	85.271	66.981	45.815	1.00	24.90
ATOM	2138	CB	SER	1165	85.812	68.401	45.981	1.00	26.62
ATOM	2139	OG	SER	1165	85.674	68.850	47.316	1.00	33.09
ATOM	2140	C	SER	1165	85.756	66.423	44.487	1.00	22.54
ATOM	2141	O	SER	1165	86.942	66.152	44.327	1.00	22.12
ATOM	2142	N	GLY	1166	84.843	66.286	43.533	1.00	21.99
ATOM	2143	CA	GLY	1166	85.184	65.741	42.232	1.00	19.49
ATOM	2144	C	GLY	1166	84.745	64.288	42.122	1.00	20.47
ATOM	2145	O	GLY	1166	84.756	63.720	41.033	1.00	19.68
ATOM	2146	N	GLY	1167	84.388	63.684	43.258	1.00	20.15
ATOM	2147	CA	GLY	1167	83.928	62.303	43.294	1.00	20.19
ATOM	2148	C	GLY	1167	82.534	62.182	42.712	1.00	20.08
ATOM	2149	O	GLY	1167	81.798	63.161	42.698	1.00	21.88
ATOM	2150	N	PRO	1168	82.109	60.986	42.297	1.00	20.02
ATOM	2151	CD	PRO	1168	82.901	59.746	42.208	1.00	20.29
ATOM	2152	CA	PRO	1168	80.786	60.792	41.710	1.00	19.44
ATOM	2153	CB	PRO	1168	81.002	59.553	40.851	1.00	21.21
ATOM	2154	CG	PRO	1168	81.880	58.729	41.726	1.00	18.35
ATOM	2155	C	PRO	1168	79.578	60.595	42.611	1.00	19.51
ATOM	2156	O	PRO	1168	79.683	60.068	43.712	1.00	20.28
ATOM	2157	N	LEU	1169	78.427	61.050	42.123	1.00	19.50
ATOM	2158	CA	LEU	1169	77.149	60.852	42.798	1.00	20.76
ATOM	2159	CB	LEU	1169	76.376	62.152	42.977	1.00	18.93
ATOM	2160	CG	LEU	1169	76.583	62.721	44.372	1.00	17.23
ATOM	2161	CD1	LEU	1169	77.483	63.924	44.272	1.00	17.53
ATOM	2162	CD2	LEU	1169	75.255	63.072	44.991	1.00	16.81
ATOM	2163	C	LEU	1169	76.444	59.952	41.807	1.00	21.18
ATOM	2164	O	LEU	1169	76.098	60.381	40.708	1.00	23.71
ATOM	2165	N	LEU	1170	76.336	58.680	42.153	1.00	21.28
ATOM	2166	CA	LEU	1170	75.736	57.702	41.267	1.00	21.46
ATOM	2167	CB	LEU	1170	76.527	56.398	41.356	1.00	17.58
ATOM	2168	CG	LEU	1170	78.027	56.488	41.086	1.00	15.37
ATOM	2169	CD1	LEU	1170	78.700	55.235	41.566	1.00	13.10

FIGURE 3 (CONT.)

ATOM	2170	CD2	LEU	1170	78.284	56.702	39.616	1.00	12.53
ATOM	2171	C	LEU	1170	74.265	57.416	41.529	1.00	24.11
ATOM	2172	O	LEU	1170	73.783	57.534	42.656	1.00	27.04
ATOM	2173	N	CYS	1171	73.540	57.104	40.466	1.00	23.89
ATOM	2174	CA	CYS	1171	72.142	56.747	40.592	1.00	26.02
ATOM	2175	CB	CYS	1171	71.421	56.978	39.265	1.00	26.82
ATOM	2176	SG	CYS	1171	71.658	55.657	38.066	1.00	28.93
ATOM	2177	C	CYS	1171	72.209	55.250	40.918	1.00	27.13
ATOM	2178	O	CYS	1171	73.285	54.648	40.840	1.00	28.91
ATOM	2179	N	PRO	1172	71.069	54.616	41.243	1.00	27.20
ATOM	2180	CD	PRO	1172	69.735	55.217	41.411	1.00	26.50
ATOM	2181	CA	PRO	1172	71.033	53.185	41.574	1.00	25.65
ATOM	2182	CB	PRO	1172	69.538	52.912	41.707	1.00	25.61
ATOM	2183	CG	PRO	1172	69.031	54.192	42.263	1.00	28.15
ATOM	2184	C	PRO	1172	71.681	52.239	40.558	1.00	25.57
ATOM	2185	O	PRO	1172	72.227	51.198	40.933	1.00	26.76
ATOM	2186	N	ALA	1173	71.606	52.576	39.277	1.00	25.34
ATOM	2187	CA	ALA	1173	72.193	51.729	38.244	1.00	25.38
ATOM	2188	CB	ALA	1173	71.454	51.915	36.936	1.00	25.17
ATOM	2189	C	ALA	1173	73.678	51.997	38.042	1.00	27.51
ATOM	2190	O	ALA	1173	74.279	51.483	37.095	1.00	29.05
ATOM	2191	N	GLY	1174	74.253	52.849	38.890	1.00	27.48
ATOM	2192	CA	GLY	1174	75.668	53.166	38.787	1.00	27.28
ATOM	2193	C	GLY	1174	76.035	54.129	37.673	1.00	26.52
ATOM	2194	O	GLY	1174	77.103	54.029	37.076	1.00	27.07
ATOM	2195	N	HIS	1175	75.140	55.047	37.353	1.00	25.55
ATOM	2196	CA	HIS	1175	75.427	56.016	36.312	1.00	25.00
ATOM	2197	CB	HIS	1175	74.313	56.027	35.281	1.00	26.94
ATOM	2198	CG	HIS	1175	74.268	54.783	34.458	1.00	27.86
ATOM	2199	CD2	HIS	1175	74.317	54.598	33.121	1.00	30.29
ATOM	2200	ND1	HIS	1175	74.228	53.525	35.018	1.00	30.38
ATOM	2201	CE1	HIS	1175	74.254	52.616	34.061	1.00	31.15
ATOM	2202	NE2	HIS	1175	74.310	53.241	32.900	1.00	31.52
ATOM	2203	C	HIS	1175	75.625	57.371	36.955	1.00	24.78
ATOM	2204	O	HIS	1175	75.027	57.656	37.990	1.00	27.48
ATOM	2205	N	ALA	1176	76.473	58.198	36.358	1.00	23.70
ATOM	2206	CA	ALA	1176	76.782	59.506	36.913	1.00	21.48
ATOM	2207	CB	ALA	1176	77.996	60.107	36.210	1.00	20.07
ATOM	2208	C	ALA	1176	75.630	60.492	36.910	1.00	21.16
ATOM	2209	O	ALA	1176	75.016	60.740	35.881	1.00	21.05
ATOM	2210	N	VAL	1177	75.339	61.036	38.083	1.00	20.47
ATOM	2211	CA	VAL	1177	74.286	62.025	38.254	1.00	20.12
ATOM	2212	CB	VAL	1177	73.375	61.663	39.454	1.00	22.63
ATOM	2213	CG1	VAL	1177	72.432	62.818	39.789	1.00	21.63
ATOM	2214	CG2	VAL	1177	72.574	60.399	39.141	1.00	20.84
ATOM	2215	C	VAL	1177	74.933	63.402	38.469	1.00	20.43
ATOM	2216	O	VAL	1177	74.374	64.436	38.086	1.00	19.45
ATOM	2217	N	GLY	1178	76.136	63.409	39.035	1.00	20.41
ATOM	2218	CA	GLY	1178	76.836	64.661	39.267	1.00	18.90
ATOM	2219	C	GLY	1178	78.153	64.429	39.972	1.00	18.98
ATOM	2220	O	GLY	1178	78.499	63.283	40.271	1.00	19.19

FIGURE 3 (CONT.)

ATOM	2221	N	LEU	1179	78.887	65.508	40.230	1.00	18.30
ATOM	2222	CA	LEU	1179	80.173	65.435	40.919	1.00	18.00
ATOM	2223	CB	LEU	1179	81.298	66.027	40.054	1.00	12.80
ATOM	2224	CG	LEU	1179	81.484	65.535	38.614	1.00	12.14
ATOM	2225	CD1	LEU	1179	82.733	66.154	38.040	1.00	9.04
ATOM	2226	CD2	LEU	1179	81.568	64.034	38.557	1.00	11.17
ATOM	2227	C	LEU	1179	80.058	66.223	42.221	1.00	18.90
ATOM	2228	O	LEU	1179	79.564	67.344	42.223	1.00	23.62
ATOM	2229	N	PHE	1180	80.476	65.632	43.332	1.00	19.19
ATOM	2230	CA	PHE	1180	80.418	66.301	44.625	1.00	19.90
ATOM	2231	CB	PHE	1180	80.994	65.370	45.692	1.00	18.26
ATOM	2232	CG	PHE	1180	81.071	65.968	47.070	1.00	18.11
ATOM	2233	CD1	PHE	1180	82.281	66.015	47.752	1.00	18.51
ATOM	2234	CD2	PHE	1180	79.936	66.426	47.714	1.00	18.19
ATOM	2235	CE1	PHE	1180	82.357	66.504	49.054	1.00	15.60
ATOM	2236	CE2	PHE	1180	80.013	66.916	49.020	1.00	18.73
ATOM	2237	CZ	PHE	1180	81.226	66.951	49.683	1.00	14.64
ATOM	2238	C	PHE	1180	81.225	67.594	44.552	1.00	21.74
ATOM	2239	O	PHE	1180	82.397	67.565	44.195	1.00	23.00
ATOM	2240	N	ARG	1181	80.583	68.727	44.826	1.00	24.80
ATOM	2241	CA	ARG	1181	81.270	70.020	44.800	1.00	26.34
ATOM	2242	CB	ARG	1181	80.427	71.116	44.144	1.00	26.66
ATOM	2243	CG	ARG	1181	81.215	72.411	43.959	1.00	29.11
ATOM	2244	CD	ARG	1181	80.365	73.532	43.425	1.00	33.23
ATOM	2245	NE	ARG	1181	79.368	73.951	44.403	1.00	39.30
ATOM	2246	CZ	ARG	1181	78.054	73.952	44.189	1.00	41.81
ATOM	2247	NH1	ARG	1181	77.559	73.555	43.020	1.00	42.79
ATOM	2248	NH2	ARG	1181	77.231	74.345	45.158	1.00	44.71
ATOM	2249	C	ARG	1181	81.636	70.475	46.200	1.00	26.61
ATOM	2250	O	ARG	1181	82.801	70.745	46.485	1.00	29.02
ATOM	2251	N	ALA	1182	80.641	70.572	47.069	1.00	26.67
ATOM	2252	CA	ALA	1182	80.892	71.008	48.426	1.00	27.49
ATOM	2253	CB	ALA	1182	80.867	72.513	48.493	1.00	29.65
ATOM	2254	C	ALA	1182	79.855	70.427	49.358	1.00	28.32
ATOM	2255	O	ALA	1182	78.764	70.072	48.926	1.00	28.73
ATOM	2256	N	ALA	1183	80.200	70.327	50.634	1.00	28.98
ATOM	2257	CA	ALA	1183	79.281	69.787	51.622	1.00	32.58
ATOM	2258	CB	ALA	1183	80.030	68.926	52.633	1.00	33.65
ATOM	2259	C	ALA	1183	78.544	70.906	52.333	1.00	34.36
ATOM	2260	O	ALA	1183	79.093	71.991	52.541	1.00	34.73
ATOM	2261	N	VAL	1184	77.290	70.635	52.680	1.00	36.46
ATOM	2262	CA	VAL	1184	76.437	71.577	53.388	1.00	37.51
ATOM	2263	CB	VAL	1184	75.019	71.572	52.816	1.00	36.89
ATOM	2264	CG1	VAL	1184	74.119	72.441	53.663	1.00	36.81
ATOM	2265	CG2	VAL	1184	75.033	72.041	51.373	1.00	36.21
ATOM	2266	C	VAL	1184	76.375	71.110	54.830	1.00	39.28
ATOM	2267	O	VAL	1184	75.844	70.041	55.116	1.00	39.09
ATOM	2268	N	CYS	1185	76.875	71.927	55.744	1.00	44.38
ATOM	2269	CA	CYS	1185	76.895	71.546	57.148	1.00	48.30
ATOM	2270	CB	CYS	1185	78.232	70.868	57.450	1.00	51.20
ATOM	2271	SG	CYS	1185	79.678	71.835	56.911	1.00	61.55

ATOM 2272	C	CYS	1185	76.654	72.660	58.166	1.00	47.66
ATOM 2273	O	CYS	1185	76.474	73.830	57.821	1.00	48.84
ATOM 2274	N	ALA	1186	76.674	72.263	59.432	1.00	46.42
ATOM 2275	CA	ALA	1186	76.482	73.153	60.563	1.00	45.62
ATOM 2276	CB	ALA	1186	75.005	73.436	60.755	1.00	46.93
ATOM 2277	C	ALA	1186	77.026	72.370	61.748	1.00	45.29
ATOM 2278	O	ALA	1186	76.737	71.184	61.888	1.00	44.78
ATOM 2279	N	ARG	1187	77.857	73.014	62.563	1.00	44.52
ATOM 2280	CA	ARG	1187	78.468	72.364	63.726	1.00	43.45
ATOM 2281	CB	ARG	1187	77.415	71.680	64.617	1.00	45.37
ATOM 2282	CG	ARG	1187	76.904	72.544	65.761	1.00	46.88
ATOM 2283	CD	ARG	1187	76.224	73.789	65.243	1.00	49.61
ATOM 2284	NE	ARG	1187	76.134	74.839	66.250	1.00	49.41
ATOM 2285	CZ	ARG	1187	75.294	75.867	66.178	1.00	50.80
ATOM 2286	NH1	ARG	1187	74.461	75.988	65.148	1.00	50.93
ATOM 2287	NH2	ARG	1187	75.280	76.772	67.146	1.00	50.83
ATOM 2288	C	ARG	1187	79.510	71.347	63.290	1.00	41.49
ATOM 2289	O	ARG	1187	79.995	70.557	64.098	1.00	43.20
ATOM 2290	N	GLY	1188	79.879	71.389	62.015	1.00	38.92
ATOM 2291	CA	GLY	1188	80.864	70.451	61.515	1.00	36.42
ATOM 2292	C	GLY	1188	80.282	69.107	61.126	1.00	34.79
ATOM 2293	O	GLY	1188	81.029	68.157	60.914	1.00	37.40
ATOM 2294	N	VAL	1189	78.960	69.014	61.037	1.00	32.66
ATOM 2295	CA	VAL	1189	78.303	67.771	60.653	1.00	30.43
ATOM 2296	CB	VAL	1189	77.228	67.334	61.689	1.00	31.40
ATOM 2297	CG1	VAL	1189	76.468	66.111	61.199	1.00	31.51
ATOM 2298	CG2	VAL	1189	77.872	67.017	63.018	1.00	33.33
ATOM 2299	C	VAL	1189	77.628	68.016	59.311	1.00	31.53
ATOM 2300	O	VAL	1189	76.740	68.867	59.203	1.00	31.66
ATOM 2301	N	ALA	1190	78.101	67.315	58.285	1.00	30.61
ATOM 2302	CA	ALA	1190	77.567	67.420	56.932	1.00	29.84
ATOM 2303	CB	ALA	1190	78.511	66.754	55.956	1.00	29.82
ATOM 2304	C	ALA	1190	76.198	66.760	56.856	1.00	31.17
ATOM 2305	O	ALA	1190	76.073	65.552	57.075	1.00	33.60
ATOM 2306	N	ALA	1191	75.174	67.545	56.542	1.00	29.63
ATOM 2307	CA	ALA	1191	73.821	67.021	56.443	1.00	27.51
ATOM 2308	CB	ALA	1191	72.880	67.836	57.313	1.00	27.97
ATOM 2309	C	ALA	1191	73.334	66.997	55.000	1.00	28.18
ATOM 2310	O	ALA	1191	72.409	66.253	54.668	1.00	31.13
ATOM 2311	N	ALA	1192	73.962	67.793	54.138	1.00	26.71
ATOM 2312	CA	ALA	1192	73.594	67.853	52.721	1.00	24.73
ATOM 2313	CB	ALA	1192	72.674	69.024	52.449	1.00	25.63
ATOM 2314	C	ALA	1192	74.858	68.002	51.909	1.00	24.75
ATOM 2315	O	ALA	1192	75.935	68.200	52.473	1.00	23.68
ATOM 2316	N	VAL	1193	74.738	67.893	50.591	1.00	25.76
ATOM 2317	CA	VAL	1193	75.897	68.017	49.712	1.00	26.76
ATOM 2318	CB	VAL	1193	76.503	66.627	49.325	1.00	27.03
ATOM 2319	CG1	VAL	1193	76.940	65.861	50.566	1.00	26.31
ATOM 2320	CG2	VAL	1193	75.512	65.807	48.515	1.00	27.41
ATOM 2321	C	VAL	1193	75.569	68.756	48.425	1.00	27.01
ATOM 2322	O	VAL	1193	74.608	68.413	47.735	1.00	27.50

FIGURE 3 (CONT.)

ATOM	2323	N	ASP	1194	76.333	69.807	48.146	1.00	26.41
ATOM	2324	CA	ASP	1194	76.180	70.587	46.926	1.00	27.71
ATOM	2325	CB	ASP	1194	76.750	71.995	47.109	1.00	30.91
ATOM	2326	CG	ASP	1194	75.836	72.906	47.907	1.00	34.47
ATOM	2327	OD1	ASP	1194	76.335	73.953	48.389	1.00	36.98
ATOM	2328	OD2	ASP	1194	74.626	72.590	48.041	1.00	35.44
ATOM	2329	C	ASP	1194	76.958	69.895	45.817	1.00	26.97
ATOM	2330	O	ASP	1194	78.163	69.650	45.964	1.00	26.74
ATOM	2331	N	PHE	1195	76.296	69.608	44.701	1.00	24.78
ATOM	2332	CA	PHE	1195	76.976	68.948	43.599	1.00	23.72
ATOM	2333	CB	PHE	1195	76.625	67.458	43.546	1.00	23.09
ATOM	2334	CG	PHE	1195	75.185	67.171	43.244	1.00	21.65
ATOM	2335	CD1	PHE	1195	74.748	67.042	41.933	1.00	21.20
ATOM	2336	CD2	PHE	1195	74.268	66.991	44.276	1.00	22.38
ATOM	2337	CE1	PHE	1195	73.417	66.736	41.650	1.00	20.66
ATOM	2338	CE2	PHE	1195	72.935	66.684	44.005	1.00	21.40
ATOM	2339	CZ	PHE	1195	72.510	66.556	42.689	1.00	21.45
ATOM	2340	C	PHE	1195	76.755	69.592	42.244	1.00	24.27
ATOM	2341	O	PHE	1195	75.898	70.452	42.076	1.00	26.48
ATOM	2342	N	ILE	1196	77.572	69.181	41.285	1.00	23.52
ATOM	2343	CA	ILE	1196	77.521	69.679	39.925	1.00	22.71
ATOM	2344	CB	ILE	1196	78.946	69.790	39.354	1.00	22.75
ATOM	2345	CG2	ILE	1196	78.903	70.308	37.923	1.00	24.48
ATOM	2346	CG1	ILE	1196	79.804	70.682	40.255	1.00	21.53
ATOM	2347	CD1	ILE	1196	81.283	70.593	39.987	1.00	20.43
ATOM	2348	C	ILE	1196	76.753	68.658	39.090	1.00	24.50
ATOM	2349	O	ILE	1196	77.240	67.552	38.856	1.00	25.41
ATOM	2350	N	PRO	1197	75.525	68.993	38.666	1.00	24.80
ATOM	2351	CD	PRO	1197	74.778	70.230	38.940	1.00	24.02
ATOM	2352	CA	PRO	1197	74.718	68.076	37.858	1.00	24.02
ATOM	2353	CB	PRO	1197	73.466	68.900	37.571	1.00	21.87
ATOM	2354	CG	PRO	1197	73.360	69.780	38.748	1.00	21.74
ATOM	2355	C	PRO	1197	75.444	67.751	36.557	1.00	24.76
ATOM	2356	O	PRO	1197	76.143	68.606	36.011	1.00	25.57
ATOM	2357	N	VAL	1198	75.267	66.537	36.044	1.00	26.89
ATOM	2358	CA	VAL	1198	75.923	66.159	34.797	1.00	28.24
ATOM	2359	CB	VAL	1198	75.541	64.746	34.338	1.00	27.91
ATOM	2360	CG1	VAL	1198	76.318	64.392	33.091	1.00	32.68
ATOM	2361	CG2	VAL	1198	75.869	63.747	35.401	1.00	28.52
ATOM	2362	C	VAL	1198	75.583	67.148	33.684	1.00	29.68
ATOM	2363	O	VAL	1198	76.397	67.390	32.794	1.00	31.51
ATOM	2364	N	ALA	1199	74.394	67.741	33.754	1.00	30.96
ATOM	2365	CA	ALA	1199	73.954	68.718	32.759	1.00	28.72
ATOM	2366	CB	ALA	1199	72.610	69.294	33.157	1.00	30.86
ATOM	2367	C	ALA	1199	74.970	69.838	32.603	1.00	27.35
ATOM	2368	O	ALA	1199	75.193	70.346	31.503	1.00	27.43
ATOM	2369	N	ASN	1200	75.593	70.223	33.707	1.00	25.52
ATOM	2370	CA	ASN	1200	76.586	71.280	33.671	1.00	25.79
ATOM	2371	CB	ASN	1200	76.951	71.723	35.084	1.00	25.77
ATOM	2372	CG	ASN	1200	75.810	72.442	35.789	1.00	27.58
ATOM	2373	OD1	ASN	1200	76.015	73.075	36.828	1.00	29.86

FIGURE 3 (CONT.)

ATOM 2374	ND2	ASN	1200	74.602	72.337	35.246	1.00	25.16
ATOM 2375	C	ASN	1200	77.828	70.842	32.907	1.00	26.50
ATOM 2376	O	ASN	1200	78.544	71.681	32.358	1.00	25.46
ATOM 2377	N	LEU	1201	78.063	69.531	32.844	1.00	27.79
ATOM 2378	CA	LEU	1201	79.213	68.977	32.125	1.00	27.44
ATOM 2379	CB	LEU	1201	79.400	67.488	32.437	1.00	27.76
ATOM 2380	CG	LEU	1201	79.560	67.059	33.897	1.00	27.52
ATOM 2381	CD1	LEU	1201	79.793	65.564	33.955	1.00	28.46
ATOM 2382	CD2	LEU	1201	80.703	67.790	34.548	1.00	24.26
ATOM 2383	C	LEU	1201	79.021	69.163	30.627	1.00	26.96
ATOM 2384	O	LEU	1201	79.891	69.694	29.946	1.00	26.74
ATOM 2385	N	GLU	1202	77.864	68.752	30.125	1.00	27.76
ATOM 2386	CA	GLU	1202	77.555	68.886	28.703	1.00	30.15
ATOM 2387	CB	GLU	1202	76.207	68.237	28.404	1.00	35.17
ATOM 2388	CG	GLU	1202	75.915	68.080	26.912	1.00	42.07
ATOM 2389	CD	GLU	1202	76.742	66.985	26.247	1.00	45.05
ATOM 2390	OE1	GLU	1202	76.867	65.882	26.837	1.00	45.05
ATOM 2391	OE2	GLU	1202	77.253	67.232	25.129	1.00	48.05
ATOM 2392	C	GLU	1202	77.530	70.362	28.311	1.00	27.55
ATOM 2393	O	GLU	1202	77.988	70.746	27.239	1.00	26.78
ATOM 2394	N	THR	1203	76.989	71.182	29.200	1.00	27.54
ATOM 2395	CA	THR	1203	76.916	72.618	28.997	1.00	28.52
ATOM 2396	CB	THR	1203	76.183	73.278	30.168	1.00	29.70
ATOM 2397	OG1	THR	1203	74.814	72.848	30.179	1.00	31.63
ATOM 2398	CG2	THR	1203	76.248	74.787	30.066	1.00	30.94
ATOM 2399	C	THR	1203	78.336	73.175	28.923	1.00	30.35
ATOM 2400	O	THR	1203	78.630	74.038	28.099	1.00	31.87
ATOM 2401	N	THR	1204	79.204	72.693	29.810	1.00	30.89
ATOM 2402	CA	THR	1204	80.597	73.126	29.839	1.00	30.06
ATOM 2403	CB	THR	1204	81.325	72.545	31.070	1.00	27.84
ATOM 2404	OG1	THR	1204	80.789	73.148	32.254	1.00	28.92
ATOM 2405	CG2	THR	1204	82.823	72.804	31.010	1.00	26.94
ATOM 2406	C	THR	1204	81.329	72.732	28.551	1.00	31.06
ATOM 2407	O	THR	1204	82.238	73.435	28.113	1.00	31.97
ATOM 2408	N	MET	1205	80.918	71.622	27.940	1.00	30.02
ATOM 2409	CA	MET	1205	81.545	71.155	26.710	1.00	29.36
ATOM 2410	CB	MET	1205	81.286	69.670	26.503	1.00	26.89
ATOM 2411	CG	MET	1205	81.846	68.816	27.605	1.00	26.79
ATOM 2412	SD	MET	1205	81.869	67.096	27.164	1.00	25.34
ATOM 2413	CE	MET	1205	80.165	66.684	27.336	1.00	26.80
ATOM 2414	C	MET	1205	81.101	71.927	25.480	1.00	30.12
ATOM 2415	O	MET	1205	81.795	71.910	24.463	1.00	31.11
ATOM 2416	N	ARG	1206	79.944	72.582	25.560	1.00	32.04
ATOM 2417	CA	ARG	1206	79.425	73.372	24.443	1.00	32.33
ATOM 2418	CB	ARG	1206	77.898	73.466	24.509	1.00	33.91
ATOM 2419	CG	ARG	1206	77.180	72.147	24.315	1.00	36.45
ATOM 2420	CD	ARG	1206	75.689	72.368	24.083	1.00	39.82
ATOM 2421	NE	ARG	1206	74.994	72.858	25.274	1.00	44.02
ATOM 2422	CZ	ARG	1206	74.337	72.082	26.140	1.00	44.21
ATOM 2423	NH1	ARG	1206	74.272	70.767	25.962	1.00	41.77
ATOM 2424	NH2	ARG	1206	73.760	72.623	27.207	1.00	44.77

| ATOM | 2425 | C | ARG | 1206 | 80.030 | 74.780 | 24.404 | 1.00 | 31.71 |
| ATOM | 2426 | O | ARG | 1206 | 80.163 | 75.405 | 25.487 | 1.00 | 33.75 |

sNS4ACOORDINATES   (Complex B)

	Atom Type	Resid	#	X	Y	Z	OCC	B	
ATOM	2535	CB	LYS	1677	101.069	76.195	38.823	1.00	42.61
ATOM	2536	CG	LYS	1677	100.696	76.412	40.284	1.00	45.42
ATOM	2537	CD	LYS	1677	99.373	77.170	40.435	1.00	48.57
ATOM	2538	CE	LYS	1677	99.221	77.735	41.859	1.00	50.16
ATOM	2539	NZ	LYS	1677	97.898	78.400	42.112	1.00	51.22
ATOM	2540	C	LYS	1677	102.635	74.294	38.331	1.00	39.53
ATOM	2541	O	LYS	1677	102.747	73.868	37.171	1.00	39.44
ATOM	2542	N	LYS	1677	103.162	76.602	37.521	1.00	40.63
ATOM	2543	CA	LYS	1677	102.536	75.793	38.615	1.00	40.89
ATOM	2544	N	GLY	1678	102.595	73.497	39.393	1.00	37.81
ATOM	2545	CA	GLY	1678	102.708	72.057	39.240	1.00	34.76
ATOM	2546	C	GLY	1678	101.509	71.417	38.576	1.00	31.90
ATOM	2547	O	GLY	1678	100.461	72.045	38.430	1.00	31.54
ATOM	2548	N	SER	1679	101.684	70.181	38.126	1.00	28.52
ATOM	2549	CA	SER	1679	100.606	69.443	37.497	1.00	25.57
ATOM	2550	CB	SER	1679	101.167	68.417	36.506	1.00	26.14
ATOM	2551	OG	SER	1679	101.609	69.016	35.303	1.00	24.59
ATOM	2552	C	SER	1679	99.807	68.703	38.562	1.00	24.40
ATOM	2553	O	SER	1679	100.280	68.506	39.688	1.00	24.38
ATOM	2554	N	VAL	1680	98.574	68.346	38.219	1.00	23.52
ATOM	2555	CA	VAL	1680	97.724	67.576	39.106	1.00	21.39
ATOM	2556	CB	VAL	1680	96.252	67.694	38.697	1.00	21.22
ATOM	2557	CG1	VAL	1680	95.392	66.728	39.493	1.00	19.38
ATOM	2558	CG2	VAL	1680	95.784	69.112	38.932	1.00	21.01
ATOM	2559	C	VAL	1680	98.230	66.158	38.894	1.00	20.14
ATOM	2560	O	VAL	1680	98.478	65.754	37.754	1.00	18.28
ATOM	2561	N	VAL	1681	98.463	65.442	39.990	1.00	20.40
ATOM	2562	CA	VAL	1681	98.990	64.085	39.922	1.00	20.62
ATOM	2563	CB	VAL	1681	100.343	63.971	40.678	1.00	18.90
ATOM	2564	CG1	VAL	1681	100.968	62.616	40.454	1.00	19.40
ATOM	2565	CG2	VAL	1681	101.283	65.039	40.231	1.00	20.79
ATOM	2566	C	VAL	1681	98.050	63.055	40.522	1.00	21.25
ATOM	2567	O	VAL	1681	97.459	63.277	41.584	1.00	19.23
ATOM	2568	N	ILE	1682	97.956	61.910	39.850	1.00	22.25
ATOM	2569	CA	ILE	1682	97.134	60.795	40.304	1.00	22.27
ATOM	2570	CB	ILE	1682	96.791	59.853	39.125	1.00	18.88
ATOM	2571	CG2	ILE	1682	96.052	58.633	39.627	1.00	19.14
ATOM	2572	CG1	ILE	1682	95.940	60.597	38.094	1.00	17.33
ATOM	2573	CD1	ILE	1682	95.611	59.800	36.862	1.00	14.03
ATOM	2574	C	ILE	1682	97.926	60.028	41.376	1.00	23.98
ATOM	2575	O	ILE	1682	98.998	59.474	41.090	1.00	24.49
ATOM	2576	N	VAL	1683	97.425	60.045	42.611	1.00	24.04
ATOM	2577	CA	VAL	1683	98.074	59.345	43.724	1.00	22.87

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FIGURE 3 (CONT.)

ATOM 2578	CB	VAL	1683	98.294	60.273	44.960	1.00	20.49
ATOM 2579	CG1	VAL	1683	99.218	61.422	44.602	1.00	21.14
ATOM 2580	CG2	VAL	1683	96.986	60.787	45.493	1.00	15.48
ATOM 2581	C	VAL	1683	97.319	58.086	44.177	1.00	22.99
ATOM 2582	O	VAL	1683	97.667	57.470	45.190	1.00	25.32
ATOM 2583	N	GLY	1684	96.294	57.704	43.423	1.00	22.53
ATOM 2584	CA	GLY	1684	95.515	56.527	43.757	1.00	21.02
ATOM 2585	C	GLY	1684	94.291	56.452	42.870	1.00	21.67
ATOM 2586	O	GLY	1684	94.144	57.267	41.956	1.00	21.86
ATOM 2587	N	ARG	1685	93.399	55.507	43.154	1.00	22.35
ATOM 2588	CA	ARG	1685	92.177	55.327	42.369	1.00	19.90
ATOM 2589	CB	ARG	1685	92.449	54.463	41.150	1.00	20.04
ATOM 2590	CG	ARG	1685	93.003	53.105	41.516	1.00	22.48
ATOM 2591	CD	ARG	1685	93.157	52.240	40.296	1.00	26.67
ATOM 2592	NE	ARG	1685	94.237	51.271	40.446	1.00	28.97
ATOM 2593	CZ	ARG	1685	95.485	51.487	40.048	1.00	27.79
ATOM 2594	NH1	ARG	1685	95.815	52.632	39.474	1.00	27.86
ATOM 2595	NH2	ARG	1685	96.404	50.557	40.224	1.00	29.00
ATOM 2596	C	ARG	1685	91.113	54.636	43.185	1.00	20.01
ATOM 2597	O	ARG	1685	91.404	54.035	44.218	1.00	22.88
ATOM 2598	N	ILE	1686	89.882	54.703	42.697	1.00	18.51
ATOM 2599	CA	ILE	1686	88.745	54.066	43.346	1.00	17.38
ATOM 2600	CB	ILE	1686	87.823	55.120	43.985	1.00	15.63
ATOM 2601	CG2	ILE	1686	86.464	54.533	44.292	1.00	14.38
ATOM 2602	CG1	ILE	1686	88.496	55.665	45.251	1.00	14.48
ATOM 2603	CD1	ILE	1686	87.740	56.758	45.935	1.00	14.17
ATOM 2604	C	ILE	1686	88.043	53.247	42.268	1.00	17.71
ATOM 2605	O	ILE	1686	87.699	53.769	41.205	1.00	17.73
ATOM 2606	N	VAL	1687	87.945	51.940	42.484	1.00	16.52
ATOM 2607	CA	VAL	1687	87.325	51.073	41.493	1.00	14.59
ATOM 2608	CB	VAL	1687	88.152	49.810	41.237	1.00	13.39
ATOM 2609	CG1	VAL	1687	87.509	48.980	40.145	1.00	11.21
ATOM 2610	CG2	VAL	1687	89.564	50.184	40.842	1.00	11.10
ATOM 2611	C	VAL	1687	85.922	50.681	41.874	1.00	15.40
ATOM 2612	O	VAL	1687	85.695	50.067	42.916	1.00	17.30
ATOM 2613	N	LEU	1688	84.990	51.081	41.016	1.00	16.16
ATOM 2614	CA	LEU	1688	83.566	50.827	41.171	1.00	15.94
ATOM 2615	CB	LEU	1688	82.792	52.003	40.578	1.00	14.08
ATOM 2616	CG	LEU	1688	82.936	53.300	41.365	1.00	15.70
ATOM 2617	CD1	LEU	1688	82.611	54.511	40.519	1.00	15.92
ATOM 2618	CD2	LEU	1688	82.026	53.212	42.559	1.00	18.17
ATOM 2619	C	LEU	1688	83.129	49.532	40.481	1.00	17.97
ATOM 2620	O	LEU	1688	82.209	48.856	40.939	1.00	20.09
ATOM 2621	N	SER	1689	83.826	49.174	39.406	1.00	20.02
ATOM 2622	CA	SER	1689	83.518	47.982	38.611	1.00	21.75
ATOM 2623	CB	SER	1689	84.253	48.060	37.266	1.00	23.96
ATOM 2624	OG	SER	1689	85.605	48.467	37.436	1.00	27.29
ATOM 2625	C	SER	1689	83.749	46.603	39.243	1.00	21.43
ATOM 2626	O	SER	1689	83.290	45.596	38.700	1.00	23.26
ATOM 2627	N	GLY	1690	84.465	46.547	40.364	1.00	21.24
ATOM 2628	CA	GLY	1690	84.724	45.277	41.015	1.00	19.68

FIGURE 3 (CONT.)

ATOM	2629	C	GLY	1690	83.431	44.657	41.500	1.00	21.01
ATOM	2630	O	GLY	1690	82.452	45.367	41.741	1.00	20.02
ATOM	2631	N	LYS	1691	83.419	43.334	41.618	1.00	22.40
ATOM	2632	CA	LYS	1691	82.245	42.596	42.075	1.00	25.78
ATOM	2633	CB	LYS	1691	81.621	41.838	40.901	1.00	30.22
ATOM	2634	CG	LYS	1691	81.068	42.740	39.813	1.00	38.96
ATOM	2635	CD	LYS	1691	80.651	41.947	38.575	1.00	46.14
ATOM	2636	CE	LYS	1691	80.270	42.880	37.405	1.00	49.42
ATOM	2637	NZ	LYS	1691	79.814	42.127	36.186	1.00	50.87
ATOM	2638	C	LYS	1691	82.705	41.610	43.142	1.00	25.02
ATOM	2639	O	LYS	1691	83.885	41.254	43.176	1.00	26.26
ATOM	2640	N	PRO	1692	81.796	41.167	44.031	1.00	23.86
ATOM	2641	CD	PRO	1692	80.365	41.516	44.115	1.00	25.36
ATOM	2642	CA	PRO	1692	82.157	40.217	45.088	1.00	23.51
ATOM	2643	CB	PRO	1692	80.801	39.691	45.542	1.00	23.49
ATOM	2644	CG	PRO	1692	79.954	40.911	45.451	1.00	24.91
ATOM	2645	C	PRO	1692	83.027	39.095	44.548	1.00	23.24
ATOM	2646	O	PRO	1692	82.724	38.506	43.515	1.00	25.88
ATOM	2647	N	ALA	1693	84.136	38.831	45.219	1.00	21.89
ATOM	2648	CA	ALA	1693	85.035	37.787	44.780	1.00	21.26
ATOM	2649	CB	ALA	1693	86.173	38.383	43.989	1.00	21.74
ATOM	2650	C	ALA	1693	85.568	37.089	46.000	1.00	22.42
ATOM	2651	O	ALA	1693	85.708	37.705	47.055	1.00	24.98
ATOM	2652	N	ILE	1694	85.810	35.791	45.879	1.00	22.49
ATOM	2653	CA	ILE	1694	86.342	35.020	46.989	1.00	21.65
ATOM	2654	CB	ILE	1694	86.052	33.524	46.794	1.00	20.10
ATOM	2655	CG2	ILE	1694	86.718	32.714	47.873	1.00	22.22
ATOM	2656	CG1	ILE	1694	84.539	33.293	46.829	1.00	20.16
ATOM	2657	CD1	ILE	1694	84.133	31.872	46.593	1.00	19.23
ATOM	2658	C	ILE	1694	87.832	35.311	46.999	1.00	22.06
ATOM	2659	O	ILE	1694	88.506	35.118	45.988	1.00	25.81
ATOM	2660	N	ILE	1695	88.336	35.837	48.109	1.00	21.38
ATOM	2661	CA	ILE	1695	89.748	36.181	48.194	1.00	19.73
ATOM	2662	CB	ILE	1695	90.112	36.812	49.557	1.00	16.79
ATOM	2663	CG2	ILE	1695	91.550	37.296	49.533	1.00	16.53
ATOM	2664	CG1	ILE	1695	89.209	38.009	49.853	1.00	11.03
ATOM	2665	CD1	ILE	1695	89.480	38.658	51.192	1.00	8.12
ATOM	2666	C	ILE	1695	90.596	34.943	47.947	1.00	22.82
ATOM	2667	O	ILE	1695	90.498	33.954	48.669	1.00	22.97
ATOM	2668	N	PRO	1696	91.407	34.967	46.886	1.00	26.75
ATOM	2669	CD	PRO	1696	91.564	36.085	45.940	1.00	28.08
ATOM	2670	CA	PRO	1696	92.279	33.851	46.520	1.00	30.50
ATOM	2671	CB	PRO	1696	93.080	34.418	45.354	1.00	29.24
ATOM	2672	CG	PRO	1696	92.138	35.395	44.733	1.00	28.73
ATOM	2673	C	PRO	1696	93.207	33.490	47.662	1.00	36.92
ATOM	2674	O	PRO	1696	93.659	34.371	48.402	1.00	37.43
ATOM	2675	N	LYS	1697	93.454	32.191	47.824	1.00	42.85
ATOM	2676	CA	LYS	1697	94.356	31.692	48.863	1.00	46.97
ATOM	2677	CB	LYS	1697	93.938	30.284	49.314	1.00	48.62
ATOM	2678	CG	LYS	1697	92.480	30.143	49.712	1.00	52.72
ATOM	2679	CD	LYS	1697	92.325	29.631	51.139	1.00	54.54

FIGURE 3 (CONT.)

				X	Y	Z	OCC	B		
ATOM	2680	CE	LYS	1697	90.885	29.167	51.394	1.00	56.49
ATOM	2681	NZ	LYS	1697	90.578	27.847	50.749	1.00	59.20
ATOM	2682	C	LYS	1697	95.789	31.645	48.311	1.00	48.94
ATOM	2683	O	LYS	1697	96.588	32.540	48.661	1.00	50.95

ZINC ION COORDINATES

		Atom Type	Resid	#	X	Y	Z	OCC	B		
ATOM	2684	ZN	ZN	901	71.089	51.399	51.975	1.00	29.52
ATOM	2685	ZN	ZN	902	70.157	56.302	36.264	1.00	32.22

WATERMOLECULE COORDINATES

		Atom Type	Resid	#	X	Y	Z	OCC	B
ATOM	2686	OH2	TIP3	1	80.188	51.569	51.895	1.00	14.91
ATOM	2687	OH2	TIP3	2	84.436	50.278	50.706	1.00	27.51
ATOM	2688	OH2	TIP3	3	80.360	48.626	54.069	1.00	26.47
ATOM	2689	OH2	TIP3	4	90.933	33.696	52.289	1.00	23.43
ATOM	2690	OH2	TIP3	5	72.460	27.233	53.507	1.00	26.41
ATOM	2691	OH2	TIP3	6	87.098	37.167	56.456	1.00	35.13
ATOM	2692	OH2	TIP3	7	80.196	47.990	42.389	1.00	32.46
ATOM	2693	OH2	TIP3	8	80.634	37.946	41.797	1.00	15.54
ATOM	2694	OH2	TIP3	9	91.083	45.806	52.787	1.00	17.30
ATOM	2695	OH2	TIP3	10	85.712	53.247	29.331	1.00	28.74
ATOM	2696	OH2	TIP3	11	89.054	50.366	50.031	1.00	18.47
ATOM	2697	OH2	TIP3	12	79.767	46.999	50.439	1.00	24.04
ATOM	2698	OH2	TIP3	13	79.409	63.138	26.964	1.00	33.09
ATOM	2699	OH2	TIP3	14	79.565	49.986	49.688	1.00	26.32
ATOM	2700	OH2	TIP3	15	88.908	25.285	68.030	1.00	19.71
ATOM	2701	OH2	TIP3	16	59.074	46.155	52.416	1.00	29.76
ATOM	2702	OH2	TIP3	17	83.621	37.213	41.479	1.00	44.52
ATOM	2703	OH2	TIP3	18	59.694	46.148	55.800	1.00	34.49
ATOM	2704	OH2	TIP3	19	94.223	75.564	42.730	1.00	38.61
ATOM	2705	OH2	TIP3	20	66.565	41.471	68.855	1.00	40.67
ATOM	2706	OH2	TIP3	21	94.230	39.125	44.532	1.00	37.61
ATOM	2707	OH2	TIP3	22	63.801	32.294	63.606	1.00	24.75
ATOM	2708	OH2	TIP3	23	85.565	24.399	71.908	1.00	34.81
ATOM	2709	OH2	TIP3	24	78.876	64.139	29.678	1.00	39.51
ATOM	2710	OH2	TIP3	25	82.850	28.849	47.546	1.00	25.28
ATOM	2711	OH2	TIP3	28	69.172	69.500	51.903	1.00	30.62
ATOM	2712	OH2	TIP3	29	66.988	51.499	56.187	1.00	30.20
ATOM	2713	OH2	TIP3	30	91.719	42.057	60.299	1.00	31.11
ATOM	2714	OH2	TIP3	31	77.543	29.196	41.350	1.00	55.87
ATOM	2715	OH2	TIP3	32	84.613	22.791	54.244	1.00	64.87
ATOM	2716	OH2	TIP3	33	71.143	49.227	43.011	1.00	36.07
ATOM	2717	OH2	TIP3	34	72.527	52.824	53.213	1.00	5.56
ATOM	2718	OH2	TIP3	35	80.116	46.082	38.809	1.00	44.35

FIGURE 3 (CONT.)

ATOM 2719	OH2	TIP3	36	65.304	58.306	50.404	1.00	50.48
ATOM 2720	OH2	TIP3	38	77.283	35.181	38.894	1.00	36.34
ATOM 2721	OH2	TIP3	39	67.275	62.937	39.441	1.00	39.30
ATOM 2722	OH2	TIP3	40	95.912	77.587	39.202	1.00	37.03
ATOM 2723	OH2	TIP3	41	87.028	46.815	50.178	1.00	14.09
ATOM 2724	OH2	TIP3	42	70.710	55.468	34.204	1.00	7.82
ATOM 2725	OH2	TIP3	43	87.279	67.965	49.287	1.00	23.95
ATOM 2726	OH2	TIP3	44	90.719	39.572	46.110	1.00	29.46
ATOM 2727	OH2	TIP3	45	88.956	32.992	50.562	1.00	26.01
ATOM 2728	OH2	TIP3	46	99.309	29.693	67.462	1.00	19.97
ATOM 2729	OH2	TIP3	47	99.173	61.794	37.290	1.00	31.61
ATOM 2730	OH2	TIP3	48	106.963	58.636	47.340	1.00	36.68
ATOM 2731	OH2	TIP3	49	85.142	35.133	43.034	1.00	19.23
ATOM 2732	OH2	TIP3	50	71.616	67.146	35.073	1.00	36.90
ATOM 2733	OH2	TIP3	51	75.865	23.589	68.938	1.00	31.60
ATOM 2734	OH2	TIP3	52	84.026	47.614	42.760	1.00	26.85
ATOM 2735	OH2	TIP3	53	99.401	56.479	39.758	1.00	21.95
ATOM 2736	OH2	TIP3	54	68.040	27.725	53.497	1.00	43.99
ATOM 2737	OH2	TIP3	55	78.583	39.197	40.332	1.00	24.68
ATOM 2738	OH2	TIP3	56	92.451	75.069	27.711	1.00	44.43
ATOM 2739	OH2	TIP3	57	89.623	49.854	35.111	1.00	22.90
ATOM 2740	OH2	TIP3	58	95.616	73.094	31.597	1.00	27.62
ATOM 2741	OH2	TIP3	59	86.253	47.246	59.568	1.00	24.37
ATOM 2742	OH2	TIP3	60	98.881	56.884	37.033	1.00	32.28
ATOM 2743	OH2	TIP3	61	107.913	59.670	50.434	1.00	40.73
ATOM 2744	OH2	TIP3	62	63.410	58.104	43.219	1.00	29.77
ATOM 2745	OH2	TIP3	63	99.184	62.943	48.341	1.00	52.93
ATOM 2746	OH2	TIP3	64	92.483	47.893	40.686	1.00	33.31
ATOM 2747	OH2	TIP3	65	76.471	22.799	61.366	1.00	33.07
ATOM 2748	OH2	TIP3	66	102.733	70.701	43.239	1.00	52.51
ATOM 2749	OH2	TIP3	67	94.669	46.032	46.815	1.00	31.75
ATOM 2750	OH2	TIP3	68	100.962	67.281	48.137	1.00	52.13
ATOM 2751	OH2	TIP3	69	76.478	37.405	40.145	1.00	25.79
ATOM 2752	OH2	TIP3	70	90.165	47.004	58.770	1.00	49.51
ATOM 2753	OH2	TIP3	71	89.912	38.696	43.283	1.00	41.39
ATOM 2754	OH2	TIP3	72	78.867	77.910	30.979	1.00	43.29
ATOM 2755	OH2	TIP3	73	105.807	71.061	33.955	1.00	35.91
ATOM 2756	OH2	TIP3	74	94.956	46.168	41.472	1.00	32.83
ATOM 2757	OH2	TIP3	75	81.755	20.284	64.565	1.00	36.36
ATOM 2758	OH2	TIP3	76	83.777	36.376	73.095	1.00	35.68
ATOM 2759	OH2	TIP3	77	90.384	42.253	62.669	1.00	45.35
ATOM 2760	OH2	TIP3	78	88.037	29.259	75.147	1.00	56.66
ATOM 2761	OH2	TIP3	79	101.859	65.470	26.683	1.00	39.64
ATOM 2762	OH2	TIP3	80	71.347	27.770	73.090	1.00	46.49
ATOM 2763	OH2	TIP3	81	105.055	72.336	36.481	1.00	34.57
ATOM 2764	OH2	TIP3	82	89.487	32.603	43.952	1.00	55.98
ATOM 2765	OH2	TIP3	83	82.955	70.726	51.485	1.00	31.53
ATOM 2766	OH2	TIP3	84	104.149	69.529	35.834	1.00	22.24
ATOM 2767	OH2	TIP3	87	97.144	58.485	29.113	1.00	38.50
ATOM 2768	OH2	TIP3	88	99.143	58.146	34.137	1.00	31.08
ATOM 2769	OH2	TIP3	89	93.402	76.905	45.088	1.00	58.17

FIGURE 3 (CONT.)

ATOM 2770	OH2	TIP3	91	98.629	61.636	27.795	1.00	44.47
ATOM 2771	OH2	TIP3	93	92.075	77.451	42.668	1.00	46.15
ATOM 2772	OH2	TIP3	94	94.761	55.023	38.581	1.00	43.31
ATOM 2773	OH2	TIP3	95	94.860	63.387	30.662	1.00	23.26
ATOM 2774	OH2	TIP3	97	96.495	61.394	31.222	1.00	17.95
ATOM 2775	OH2	TIP3	99	97.135	61.058	33.735	1.00	24.21
ATOM 2776	OH2	TIP3	100	98.598	62.340	24.703	1.00	15.55
ATOM 2777	OH2	TIP3	101	96.091	63.609	25.209	1.00	16.64
ATOM 2778	OH2	TIP3	102	95.591	62.210	28.267	1.00	28.35
ATOM 2779	OH2	TIP3	103	84.181	68.384	51.386	1.00	37.36
ATOM 2780	OH2	TIP3	104	90.542	76.184	46.889	1.00	50.54
ATOM 2781	OH2	TIP3	105	87.338	52.422	55.348	1.00	57.64
ATOM 2782	OH2	TIP3	106	86.485	55.114	55.782	1.00	53.13
ATOM 2783	OH2	TIP3	107	71.978	33.253	38.083	1.00	37.67
ATOM 2784	OH2	TIP3	108	86.389	52.030	52.810	1.00	45.08
ATOM 2785	OH2	TIP3	109	88.375	44.898	51.380	1.00	45.72
ATOM 2786	OH2	TIP3	110	76.040	31.693	38.282	1.00	49.11
ATOM 2787	OH2	TIP3	111	88.171	23.460	70.887	1.00	34.87
ATOM 2788	OH2	TIP3	112	81.925	26.203	48.120	1.00	34.21
ATOM 2789	OH2	TIP3	113	75.036	35.002	37.397	1.00	43.93
ATOM 2790	OH2	TIP3	114	66.842	37.170	41.543	1.00	37.92
ATOM 2791	OH2	TIP3	115	74.137	22.561	64.810	1.00	39.94
ATOM 2792	OH2	TIP3	116	75.230	29.105	47.361	1.00	33.31
ATOM 2793	OH2	TIP3	117	71.548	35.570	75.085	1.00	51.53
ATOM 2794	OH2	TIP3	118	91.190	40.939	65.032	1.00	59.85
ATOM 2795	OH2	TIP3	119	89.208	54.691	55.131	1.00	49.67
ATOM 2796	OH2	TIP3	120	87.603	20.791	70.317	1.00	41.15
ATOM 2797	OH2	TIP3	121	82.007	24.661	44.978	1.00	44.91
ATOM 2798	OH2	TIP3	122	67.254	62.385	54.134	1.00	55.45
ATOM 2799	OH2	TIP3	123	69.652	50.335	60.131	1.00	56.04
ATOM 2800	OH2	TIP3	124	91.100	35.309	64.126	1.00	10.24
ATOM 2801	OH2	TIP3	125	75.803	55.613	55.160	1.00	19.38
ATOM 2802	OH2	TIP3	126	67.414	58.406	48.372	1.00	50.59
ATOM 2803	OH2	TIP3	127	61.992	60.345	41.276	1.00	54.28
ATOM 2804	OH2	TIP3	128	100.397	72.990	35.528	1.00	47.93
ATOM 2805	OH2	TIP3	129	78.374	54.246	34.009	1.00	25.64
ATOM 2806	OH2	TIP3	130	74.448	74.269	39.281	1.00	43.21
ATOM 2807	OH2	TIP3	131	64.202	44.752	43.474	1.00	49.87
ATOM 2808	OH2	TIP3	132	88.521	75.111	27.052	1.00	58.72
ATOM 2809	OH2	TIP3	133	69.530	56.754	48.247	1.00	28.48
ATOM 2810	OH2	TIP3	134	79.780	77.649	41.569	1.00	58.74
ATOM 2811	OH2	TIP3	135	88.780	33.735	64.655	1.00	36.24
ATOM 2812	OH2	TIP3	136	104.389	57.542	20.144	1.00	59.52
ATOM 2813	OH2	TIP3	137	64.410	59.785	53.812	1.00	52.08
ATOM 2814	OH2	TIP3	138	99.184	58.625	27.266	1.00	30.88
ATOM 2815	OH2	TIP3	139	101.746	57.264	20.715	1.00	37.99

END
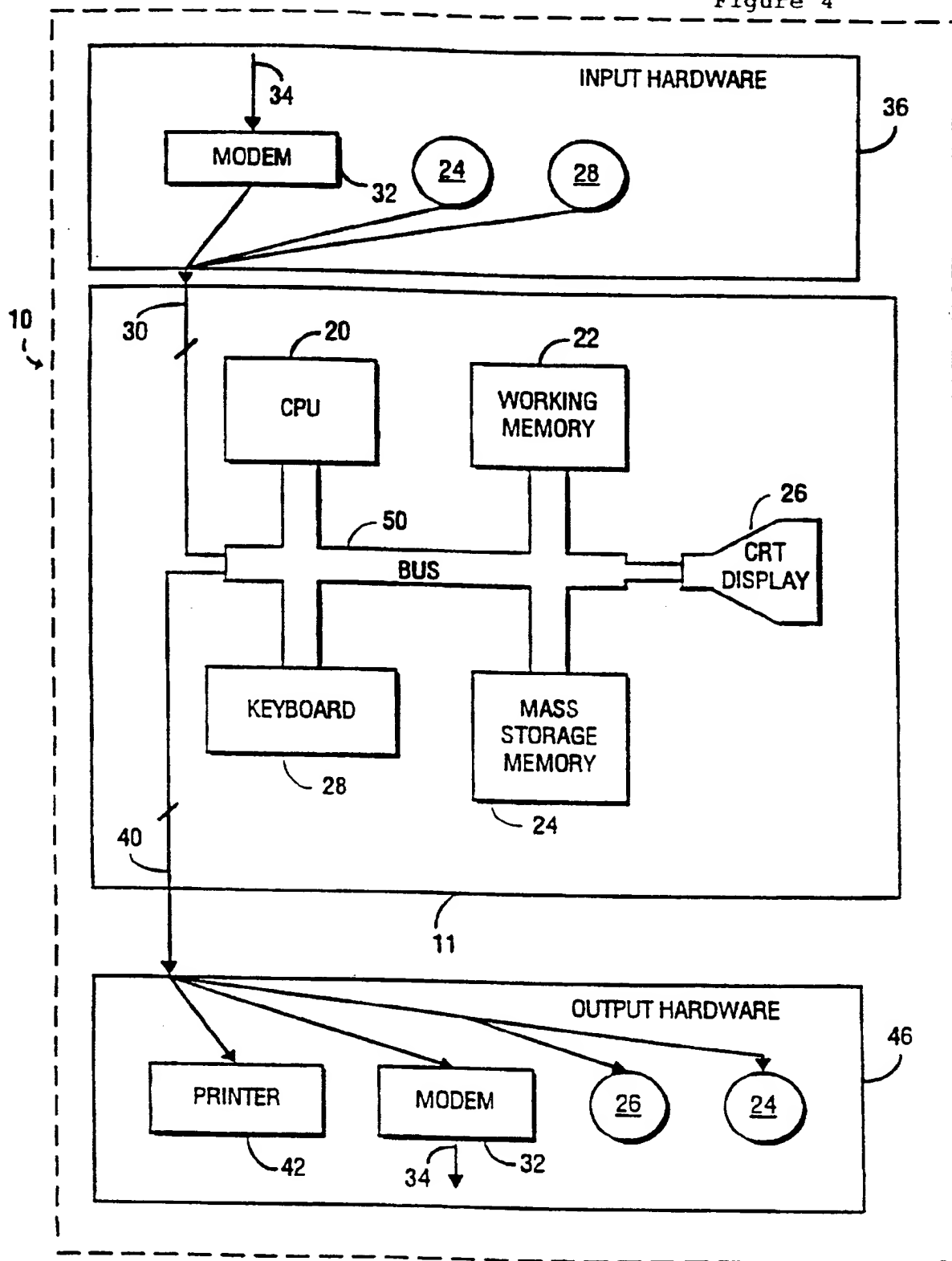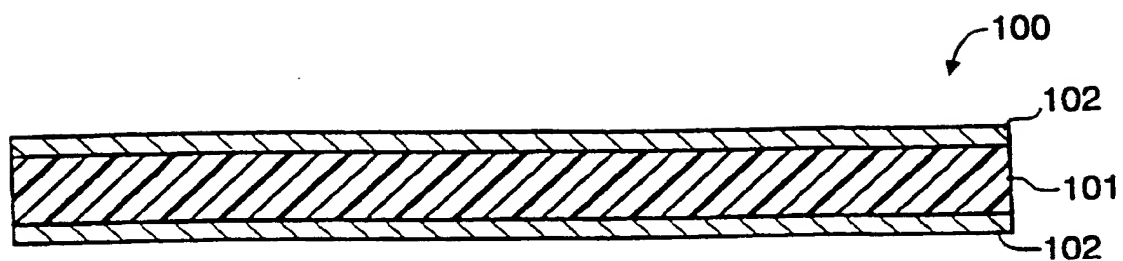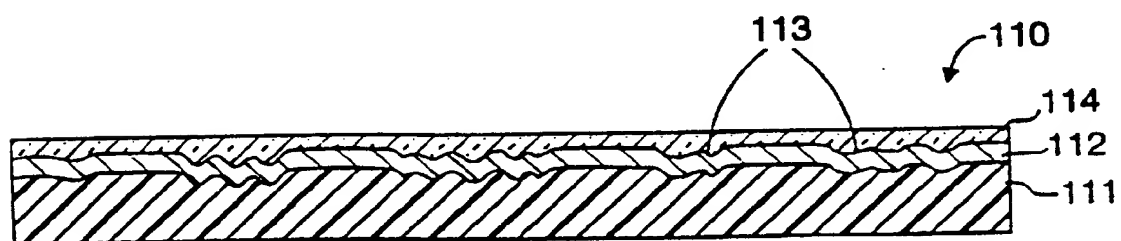
Figure 4

Figure 5

Figure 6

INTERNATIONAL SEARCH REPORT

A. CLASSIFICATION OF SUBJECT MATTER
IPC 6   C07K14/18   C07K1/00   G06F17/50   C30B7/00

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED
Minimum documentation searched (classification system followed by classification symbols)
IPC 6   C07K   G06F   C30B

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	C LIN ET AL.: "A central region in the hepatitis C virus NS4A protein allows formation of an active NS3-NS4A serine proteinase complex in vivo and in vitro" JOURNAL OF VIROLOGY., vol. 69, no. 7, July 1995, AMERICAN SOCIETY FOR MICROBIOLOGY US, pages 4373-4380, XP002053691 see the whole document --- -/--	1-3

| X | Further documents are listed in the continuation of box C. | | X | Patent family members are listed in annex. |

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"X" document of particular relevance: the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone

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"&" document member of the same patent family

Date of the actual completion of the international search	Date of mailing of the international search report
28 January 1998	13/02/1998

Name and mailing address of the ISA	Authorized officer
European Patent Office, P B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl. Fax: (+31-70) 340-3016	Masturzo, P

C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category	Citation of document. with indication,where appropriate, of the relevant passages	Relevant to claim No.
X	R BARTENSCHLAGER ET AL.: "Complex formation between the NS3 serine-type proteinase of the hepatitis C virus and NS4A and its importance for polyprotein maturation " JOURNAL OF VIROLOGY., vol. 69, no. 12, December 1995, AMERICAN SOCIETY FOR MICROBIOLOGY US, pages 7519-7528, XP002053692 see the whole document	1,2
X	WO 95 22985 A (ISTITUTO ANGELETTI) 31 August 1995 see claims 5,6	1,2
P,X	J L KIM ET AL.: "Crystal structure of the hepatitis C virus NS3 protease domain complexed with a synthetic NS4A cofactor peptide" CELL, vol. 87, 18 October 1996, NA US, pages 343-355, XP002053693 see the whole document	1-14

INTERNATIONAL SEARCH REPORT

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		EP 0746333 A	11-12-96